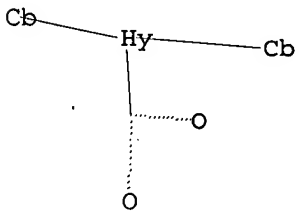
EAST Search History

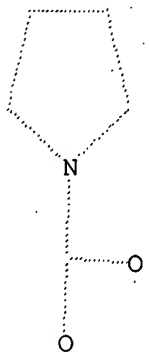
Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	77829	"544"/$$$.ccls.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/28 12:41
L2	81334	"546"/$$$.ccls.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/28 12:41
L3	82127	"548"/$$$.ccls.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/28 12:41
L4	184889	l1 or l2 or l3	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/28 12:42
L5	2689	l4 and carboxylate and pyrrole and dihydro	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/28 12:42
L6	2622	l5 and phenyl	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/28 12:43
L7	34	l6 and 2,5-dihydro-1h-pyrrole	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/28 12:44

```
=> d his

     (FILE 'HOME' ENTERED AT 09:43:01 ON 28 JUN 2007)

     FILE 'REGISTRY' ENTERED AT 09:43:39 ON 28 JUN 2007
L1             STRUCTURE UPLOADED
L2           1 S L1
L3     1680305 S NC4/ES
L4           1 S L1 SAM SUB=L3

     FILE 'STNGUIDE' ENTERED AT 09:44:40 ON 28 JUN 2007

     FILE 'REGISTRY' ENTERED AT 09:49:11 ON 28 JUN 2007
L5        2469 S L1 SSS FULL SUB=L3
L6             STRUCTURE UPLOADED
L7           2 S L6 SAM SUB=L5
L8          81 S L6 SSS FULL SUB=L5

     FILE 'CAPLUS' ENTERED AT 09:50:46 ON 28 JUN 2007
L9          46 S L8

     FILE 'REGISTRY' ENTERED AT 09:51:04 ON 28 JUN 2007

     FILE 'CAPLUS' ENTERED AT 09:51:46 ON 28 JUN 2007

     FILE 'REGISTRY' ENTERED AT 09:51:59 ON 28 JUN 2007

=> d l1
L1 HAS NO ANSWERS
L1             STR
```



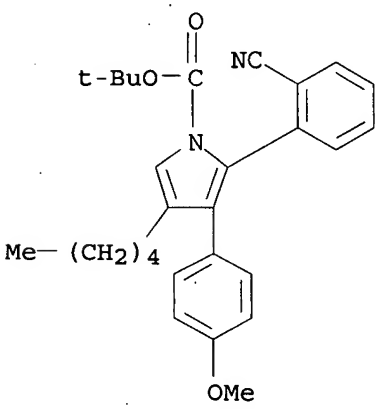
Structure attributes must be viewed using STN Express query preparation.

```
=> d l6
L6 HAS NO ANSWERS
L6             STR
```



=> d l9 tot bib abs hitstr
THE ESTIMATED COST FOR THIS REQUEST IS 242.42 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

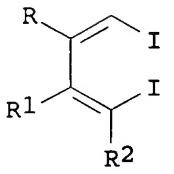
L9 ANSWER 1 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:196895 CAPLUS
DN 146:421796
TI Copper-Catalyzed Vinylation of Hydrazides. A Regioselective Entry to Highly Substituted Pyrroles
AU Rivero, Marta Rodriguez; Buchwald, Stephen L.
CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SO Organic Letters (2007), 9(6), 973-976
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
AB A modular route to highly substituted pyrroles has been developed. This transformation consists of two sequential copper-catalyzed vinylations of bis-Boc-hydrazine followed by thermal rearrangement/cyclization. A wide variety of functionalized pyrroles can be prepared in a selective manner from simple and easily accessible precursors.
IT 934424-14-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective preparation of substituted pyrroles via two sequential copper-catalyzed vinylation of hydrazide with vinyl iodides followed by rearrangement and cyclization)
RN 934424-14-3 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-(2-cyanophenyl)-3-(4-methoxyphenyl)-4-pentyl-, 1,1-dimethylethyl ester (CA INDEX NAME)



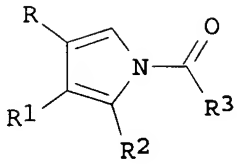
RE.CNT 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:82180 CAPLUS
DN 146:462080
TI Copper-Catalyzed Double N-Alkenylation of Amides: An Efficient Synthesis of Di- or Trisubstituted N-Acylpyrroles
AU Yuan, Xiyuan; Xu, Xiaobing; Zhou, Xiaobo; Yuan, Jiwei; Mai, Lugen; Li, Yanzhong
CS Department of Chemistry and Shanghai Key Laboratory of Green Chemistry and Chemical Processes, East China Normal University, Shanghai, 200062, Peop. Rep. China
SO Journal of Organic Chemistry (2007), 72(4), 1510-1513
CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society
DT Journal
LA English
OS CASREACT 146:462080
GI



I

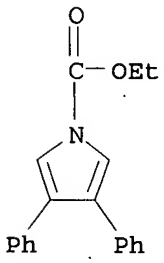


II

AB Diiodobutadienes I [R = Bu, Ph; R1 = EtCH2, Bu, Ph; R2 = H, EtCH2, Ph; RR1 = (CH2)4] undergo cyclocondensation reactions with amides R3CONH2 (R3 = Bu, PhCH2, 4-MeC6H4, 4-H2NC6H4) or Et carbamate in the presence of copper (I) iodide and trans-N,N'-dimethyl-1,2-cyclohexanediamine with cesium carbonate as the base to provide acylpyrroles II [R = Bu, Ph; R1 = EtCH2, Bu, Ph; RR1 = (CH2)4; R2 = H, EtCH2, Ph; R3 = EtO, Bu, PhCH2, 4-MeC6H4, 4-H2NC6H4] in 32-95% yields; in some cases, N-unsubstituted pyrroles are obtained as the major products. Other catalysts and bases are tried; a tetraethyldiiodobutadiene gives no product under the cyclocondensation conditions.

IT 934801-78-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of N-acylpyrroles by cyclocondensation/double alkenylation of di- and trisubstituted diiodobutadienes with primary amides in the presence of copper iodide and trans-N,N'-dimethylcyclohexanediamine with cesium carbonate as a base)

RN 934801-78-2 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 3,4-diphenyl-, ethyl ester (CA INDEX NAME)



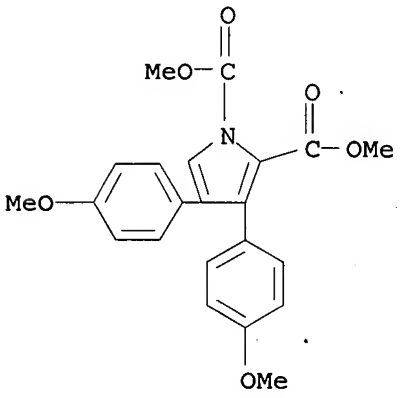
RE.CNT 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1319216 CAPLUS
DN 146:229113
TI Regioselective couplings of dibromopyrrole esters
AU Handy, Scott T.; Zhang, Yanan
CS Department of Chemistry, Binghamton University, Binghamton, NY, 13902, USA
SO Synthesis (2006), (22), 3883-3887
CODEN: SYNTBF; ISSN: 0039-7881
PB Georg Thieme Verlag
DT Journal
LA English
OS CASREACT 146:229113
AB The regioselectivity of the Suzuki couplings of several 4,5- and 3,4-dibromopyrrole-2-carboxylate esters was studied. In general,

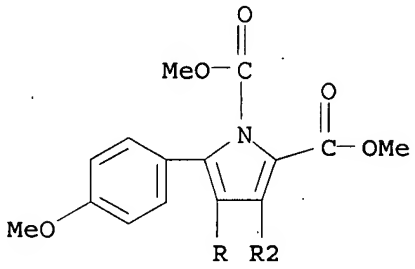
regioselectivity can be achieved for initial coupling at the more electron-deficient site (C5 and C3, resp.). At the same time, conversions are often modest (40-60%) and attempts to force the reactions to higher conversions often lead to competitive dicoupling. E.g., Suzuki coupling of 2-Et 1-Me 4,5-dibromo-1H-pyrrole-1,2-dicarboxylate with 4-methoxyphenyl boronic acid gave 2-Et 1-Me 4-bromo-5-(4-methoxyphenyl)-1H-pyrrole-1,2-dicarboxylate in 56% yield. There is some influence of steric effects on the selectivity of the reaction.

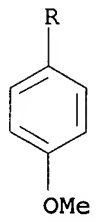
IT 924708-88-3P 924708-90-7P
RL: BYP (Byproduct); PREP (Preparation)
(regioselective Suzuki coupling of dibromopyrrole carboxylates)

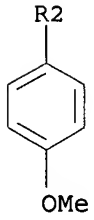
RN 924708-88-3 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3,4-bis(4-methoxyphenyl)-, 1,2-dimethyl ester (CA INDEX NAME)



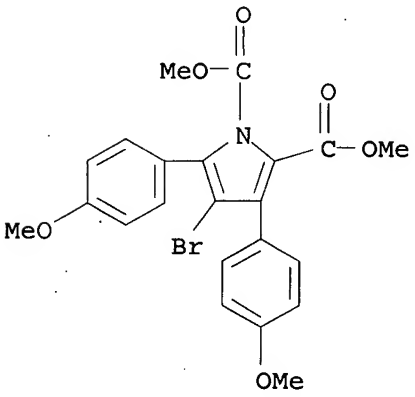
RN 924708-90-7 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3,4,5-tris(4-methoxyphenyl)-, 1,2-dimethyl ester (CA INDEX NAME)





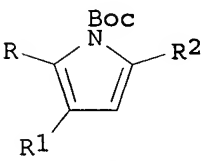


IT 924708-89-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective Suzuki coupling of dibromopyrrole carboxylates)
RN 924708-89-4 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 4-bromo-3,5-bis(4-methoxyphenyl)-, 1,2-dimethyl ester (CA INDEX NAME)

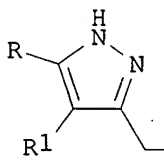


RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1224182 CAPLUS
DN 146:142558
TI Domino Cu-catalyzed C-N coupling/hydroamidation: a highly efficient synthesis of nitrogen heterocycles
AU Martin, Ruben; Rivero, Marta Rodriguez; Buchwald, Stephen L.
CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SO Angewandte Chemie, International Edition (2006), 45(42), 7079-7082
CODEN: ACIEF5; ISSN: 1433-7851
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
OS CASREACT 146:142558
GI



I



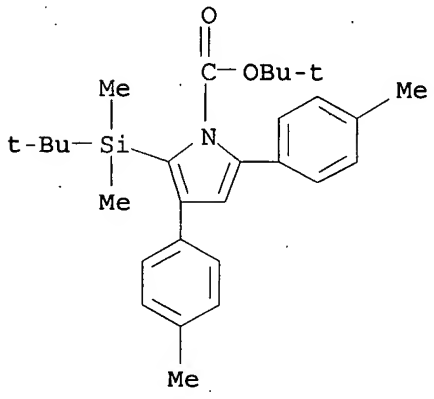
II

AB Boc-protected pyrroles and fused pyrroles and pyrazoles and fused pyrazoles with a variety of substituents are prepared by copper-catalyzed coupling and hydroamidation reactions of iodo- or bromoalkenynes and iodo- or bromoaryl alkynes with either tert-Bu carbamate or di-tert-Bu hydrazinedicarboxylate. Iodoenynes RCI:CR1C.tplbond.CR2 [R = EtCH2, Bu, Ph, 1-cyclohex-1-enyl, TIPSOCH2, MeO2C, TBS; R1 = H, EtCH2, 4-MeC6H4; RR1 = (CH2)3; R2 = H, EtCH2, Bu, BuCH2, 1-cyclohex-1-enyl, Ph, Cl(CH2)3, Me(CH2)7, 4-MeC6H4; TIPS = triisopropylsilyl; TBS = tert-butyldimethylsilyl] undergo coupling and hydroamidation reactions with BocNH2 in the presence of copper (I) iodide and N,N'-dimethylethylendiamine with cesium carbonate as a base in THF at 80° to give 1-Boc-pyrroles I [R = EtCH2, Bu, Ph, 1-cyclohex-1-enyl, TIPSOCH2, MeO2C, TBS; R1 = H, EtCH2, 4-MeC6H4; RR1 = (CH2)3; R2 = H, EtCH2, Bu, BuCH2, 1-cyclohex-1-enyl, Ph, Cl(CH2)3, Me(CH2)7, 4-MeC6H4; Boc = tert-butoxycarbonyl] in 52-95% yields; bromoenynes can be used when the reaction is performed in toluene (with potassium carbonate as the base) at 110°. Bromothienyl alkynes and an iodopyridinyl alkyne undergo copper-catalyzed cyclocondensation with tert-Bu carbamate under similar conditions to give thienopyrroles and a pyrrolopyridine, resp. Iodoenynes RCI:CR1C.tplbond.CR2 [R = H, EtCH2, Bu, Ph, PhCH2, TIPSOCH2; R1 = H, Et; RR1 = (CH2)3; R2 = H, EtCH2, BuCH2, Me(CH2)7, Ph, Cl(CH2)3, PhCH2O(CH2)2, EtO2C] undergo coupling and hydroamidation reactions with BocNH2 in the presence of copper (I) iodide and N,N'-dimethylethylendiamine with cesium carbonate as a base in THF at 80° followed by deprotection with F3CCO2H in CH2Cl2 to give pyrazoles II [R = H, EtCH2, Bu, Ph, PhCH2, TIPSOCH2; R1 = H, Et; RR1 = (CH2)3; R2 = H, EtCH2, BuCH2, Me(CH2)7, Ph, Cl(CH2)3, PhCH2O(CH2)2, EtO2C] in 66-93% yields. Ligands for the cyclocondensation are tested; only N,N'-dimethylethylenediamine and N,N'-dimethyl-trans-1,2-cyclohexanediamine are effective. The coupling and hydroamidation reactions require the presence of both the copper catalyst and ligand and added base. The prepns. of most of the iodoenyne and bromoenyne starting materials (as well as those of the bromothienyl alkynes and the iodopyridinyl alkyne) are described. Amine and hydrazine coupling products with an iodoenyne and a alkylidenedihydropyrazoledicarboxylate intermediate in the preparation of a pyrazole are isolated, supporting a coupling-hydroamidation pathway (rather than a hydroamidation-coupling pathway) for the reaction.

IT 919123-93-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrroles by copper-catalyzed cyclocondensation (coupling/hydroamidation) reactions of a carbamate with iodoenynes and bromoenynes)

RN 919123-93-6 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 2-[(1,1-dimethylethyl)dimethylsilyl]-3,5-bis(4-methylphenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



RE.CNT 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD

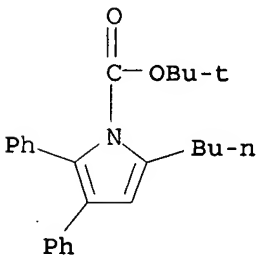
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1009616 CAPLUS
DN 145:377330
TI Methods for the synthesis of heteroaromatic compounds by immobilized silver-catalyzed 5-endo-cyclization of alkynes
IN Knight, David W.
PA University College Cardiff Consultants Limited, UK
SO PCT Int. Appl., 56pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006100479	A1	20060928	WO 2006-GB1048	20060322

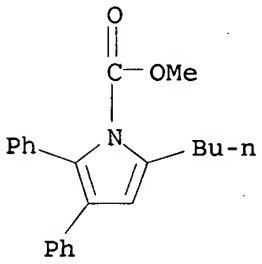
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI GB 2005-5861 A 20050322
OS CASREACT 145:377330; MARPAT 145:377330
AB Methods of making heteroarom. compds. comprising a 5-membered ring, and dihydro forms thereof, by a metal catalyzed 5-endo-cyclization of alkynes (acetylenes) are disclosed. The methods involve the use of a catalyst comprising a silver salt, more preferably a silver(I) salt, which is employed as a heterogeneous catalyst for the cyclization reaction. The methods can produce different types of heteroarom. compds. and are capable of producing highly substituted products, i.e. products in which the 5-membered ring is disubstituted, trisubstituted or, with further simple reactions, tetrasubstituted. The methods described herein generally the advantages that they use conditions and reagents that are benign, cheap and flexible and amenable to scale up, and in which the only byproduct is water.
IT 910896-29-6P 910896-30-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of heteroarom. compds. via endo-cyclization of alkynes catalyzed by immobilized silver salts)
RN 910896-29-6 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 5-butyl-2,3-diphenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 910896-30-9 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 5-butyl-2,3-diphenyl-, methyl ester (9CI) (CA INDEX NAME)

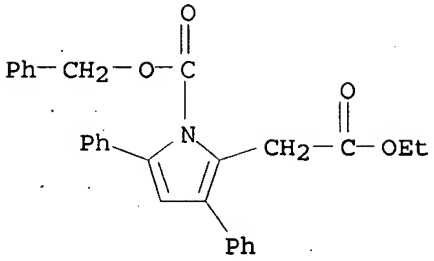


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 6 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:725314 CAPLUS
DN 145:292812
TI Efficient Synthesis of 1,3,5-Trisubstituted (Pyrrol-2-yl)acetic Acid Esters via Dual Nucleophilic Reactions of Sulfonamides or Carbamate with 4-Trimethyl-siloxy-(5E)-hexen-2-ynoates: Lewis Acid Catalyzed SN1 and Intramolecular Michael Addition
AU Ishikawa, Teruhiko; Aikawa, Toshiaki; Watanabe, Shinichiro; Saito, Seiki
CS Department of Medical and Bioengineering Science, Graduate School of Natural Science and Technology, Okayama University, Okayama, 700-8530, Japan
SO Organic Letters (2006), 8(17), 3881-3884
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
OS CASREACT 145:292812
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

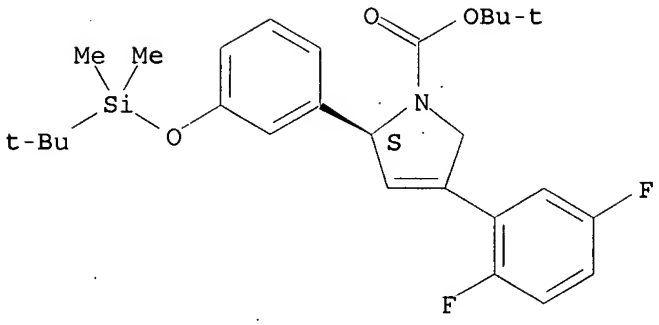
AB Benzyl carbamate or sulfonamides have proven to regioselectively attack 2-propynyl-allyl hybrid cations, generated by the action of TMSOTf on 4-(trimethylsiloxy)hex-5-en-2-ynoates, e.g., I, to afford conjugated 6-aminohex-4-en-2-ynoates, e.g., II, in which an intramol. amino-Michael reaction took place, leading to pyrroleacetates, e.g., III. The sulfonamides gave the pyrroleacetates by a one-pot process.
IT 908254-71-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrroleacetates via regioselective Lewis acid-catalyzed nucleophilic substitution of (trimethylsiloxy)hexenynoates with sulfonamides or benzyl carbamate followed by intramol. Michael addition)
RN 908254-71-7 CAPLUS
CN 1H-Pyrrole-2-acetic acid, 3,5-diphenyl-1-[(phenylmethoxy)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



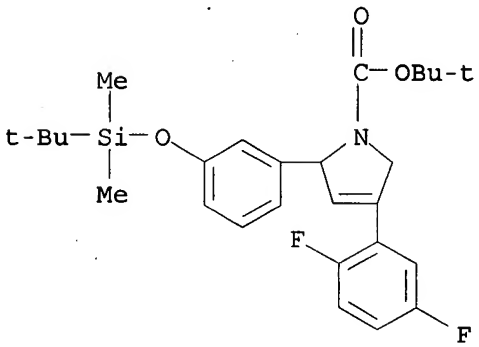
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:188863 CAPLUS
DN 144:432640
TI Kinesin spindle protein (KSP) inhibitors. Part 3: Synthesis and evaluation of phenolic 2,4-diaryl-2,5-dihydropyrroles with reduced hERG binding and employment of a phosphate prodrug strategy for aqueous solubility
AU Garbaccio, Robert M.; Fraley, Mark E.; Tasber, Edward S.; Olson, Christy M.; Hoffman, William F.; Arrington, Kenneth L.; Torrent, Maricel; Buser, Carolyn A.; Walsh, Eileen S.; Hamilton, Kelly; Schaber, Michael D.; Fernandes, Christine; Lobell, Robert B.; Tao, Weikang; South, Vicki J.; Yan, Youwei; Kuo, Lawrence C.; Prueksaritanont, Thomayant; Slaughter, Donald E.; Shu, Cathy; Heimbrook, David C.; Kohl, Nancy E.; Huber, Hans E.; Hartman, George D.
CS Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(7), 1780-1783
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 144:432640
AB 2,4-Diaryl-2,5-dihydropyrroles have been discovered to be novel, potent and water-soluble inhibitors of KSP, an emerging therapeutic target for the treatment of cancer. A potential concern for these basic KSP inhibitors was hERG binding that can be minimized by incorporation of a potency-enhancing C-2 phenol combined with neutral N-1 side chains. Aqueous solubility was restored to these, and other, non-basic inhibitors, through a phosphate prodrug strategy.
IT 884651-21-2P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2,4-diaryl-2,5-dihydropyrroles as kinesin spindle protein (KSP) inhibitors with reduced hERG binding and phosphate prodrugs for aqueous solubility)
RN 884651-21-2 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-2,5-dihydro-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

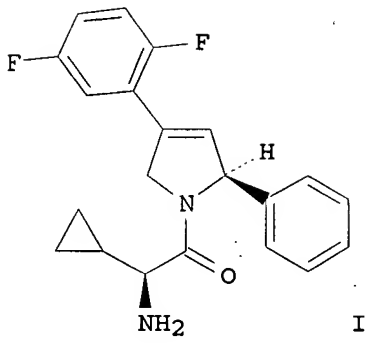


IT 639077-57-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2,4-diaryl-2,5-dihydropyrroles as kinesin spindle protein (KSP) inhibitors with reduced hERG binding and phosphate prodrugs for aqueous solubility)
RN 639077-57-9 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-2,5-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 8 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:188862 CAPLUS
DN 144:432639
TI Kinesin spindle protein (KSP) inhibitors. Part 2: The design, synthesis, and characterization of 2,4-diaryl-2,5-dihydropyrrole inhibitors of the mitotic kinesin KSP
AU Fraley, Mark E.; Garbaccio, Robert M.; Arrington, Kenneth L.; Hoffman, William F.; Tasber, Edward S.; Coleman, Paul J.; Buser, Carolyn A.; Walsh, Eileen S.; Hamilton, Kelly; Fernandes, Christine; Schaber, Michael D.; Lobell, Robert B.; Tao, Weikang; South, Victoria J.; Yan, Youwei; Kuo, Lawrence C.; Prueksaritanont, Thomayant; Shu, Cathy; Torrent, Maricel; Heimbrook, David C.; Kohl, Nancy E.; Huber, Hans E.; Hartman, George D.
CS Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(7), 1775-1779
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 144:432639
GI



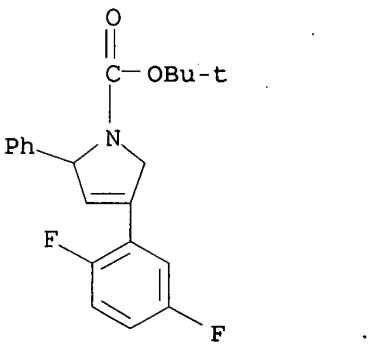
I

AB The development of nonracemic 1-acyl-2-phenyl-4-(2,5-difluorophenyl)-2,5-dihydropyrroles such as I as inhibitors of kinesin spindle protein (KSP) is described. Modification of the pyrazoline core of the lead compound to a dihydropyrrole core followed by introduction of basic amide and urea moieties yields compds. with enhanced potency and aqueous solubility which cause mitotic arrest of A2780 human ovarian carcinoma cells with EC50 values of < 10 nM. The binding of 1-acyl-2-phenyl-4-(2,5-difluorophenyl)-2,5-dihydropyrroles to KSP and to the potassium channel hERG is compared to those of the corresponding 1-acyl-5-phenyl-3-(2,5-difluorophenyl)-4,5-dihydropyrazoles. The pharmacokinetics for I in rats, dogs, and monkeys are determined Crystal structures of three dihydropyrroles bound to the allosteric site of KSP are determined by X-ray crystallog.

IT 635724-42-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-phenyl-4-(2,5-difluorophenyl)-1-acyl-2,5-dihydropyrroles and comparison of their inhibition of KSP and of mitosis and their binding selectivities for KSP over the potassium channel hERG to those of the corresponding pyrazolines)

RN 635724-42-4 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

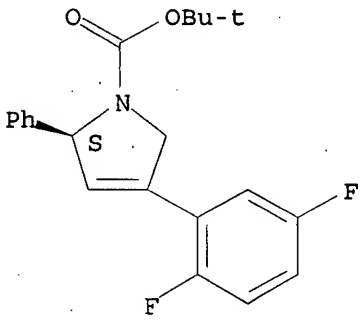


IT 635724-48-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nonracemic 2-phenyl-4-(2,5-difluorophenyl)-1-acyl-2,5-dihydropyrroles, their inhibition of KSP and of mitosis, and their binding selectivities for KSP over the potassium channel hERG)

RN 635724-48-0 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



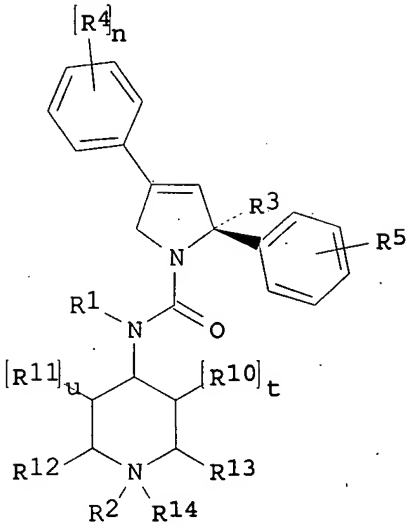
RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:182653 CAPLUS
DN 142:280064
TI Preparation of dihydropyrrolecarboxamides as mitotic kinesin inhibitors for treating cancer
IN Coleman, Paul J.; Cox, Christopher D.; Garbaccio, Robert M.; Hartman, George D.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 187 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

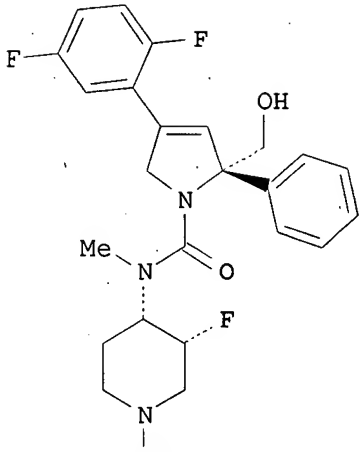
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005019206	A1	20050303	WO 2004-US26012	20040811
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2005043357	A1	20050224	US 2004-915743	20040811
	AU 2004266232	A1	20050303	AU 2004-266232	20040811
	CA 2534065	A1	20050303	CA 2004-2534065	20040811
	EP 1664026	A1	20060607	EP 2004-780791	20040811
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR				
	CN 1839128	A	20060927	CN 2004-80023309	20040811
	BR 2004013580	A	20061017	BR 2004-13580	20040811
	JP 2007502774	T	20070215	JP 2006-523332	20040811
	US 2006234984	A1	20061019	US 2006-567676	20060209
	NO 2006001194	A	20060505	NO 2006-1194	20060314
PRAI	US 2003-495637P	P	20030815		
	US 2004-563580P	P	20040419		
	US 2003-512680P	P	20031020		
	US 2004-563586P	P	20040419		
	WO 2004-US25980	W	20040811		
	WO 2004-US26012	W	20040811		

OS MARPAT 142:280064

GI



I



II

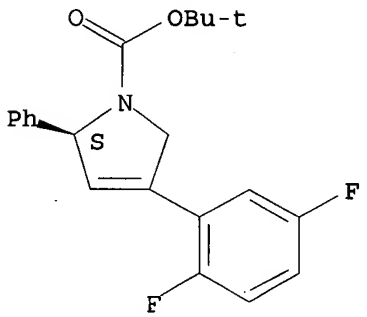
AB The present invention relates to dihydropyrrole compds. I [R1, R2 = H, alkyl, aryl, etc.; R3 = H, alkyl, CH2OH, etc.; R4 = CO2H, halo, CN, etc.; R5 = H, halo, CN, etc.; R10, R11 = F, CH2F; R12, R13 = H, CH2F; R14 = absent, oxo; n = 0-3; t = 0-2; u = 0-1] that are useful for treating cellular proliferative diseases, for treating disorders associated with KSP kinesin activity, and for inhibiting KSP kinesin. E.g., a multi-step synthesis of II, which showed an IC50 of ≤ 50 μM in kinesin ATPase in vitro assay, was given. The invention is also related to compns. which comprise these compds. I, and methods of using them to treat cancer in mammals.

IT 635724-48-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dihydropyrrolecarboxamides as mitotic kinesin inhibitors for treating or preventing cancer)

RN 635724-48-0 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 10 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:140806 CAPLUS

DN 142:240324
TI A preparation of pyrrolecarboxamide derivatives, useful as mitotic kinesin inhibitors
IN Coleman, Paul J.; Cox, Christopher D.; Garbaccio, Robert M.; Hartman, George D.
PA USA
SO U.S. Pat. Appl. Publ., 52 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005038074	A1	20050217	US 2004-916096	20040811
	WO 2005019205	A1	20050303	WO 2004-US25980	20040811
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	BR 2004013580	A	20061017	BR 2004-13580	20040811
	NO 2006001194	A	20060505	NO 2006-1194	20060314
PRAI	US 2003-495637P	P	20030815		
	US 2003-512680P	P	20031020		
	US 2004-563586P	P	20040419		
	WO 2004-US25980	W	20040811		

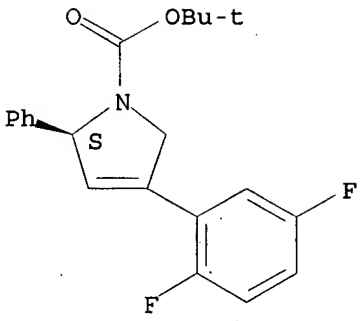
OS CASREACT 142:240324; MARPAT 142:240324
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a preparation of pyrrolecarboxamide derivs. of formula I [wherein: R1 is H, alkyl, aryl, or heterocyclyl, etc.; R2 is 4-piperidinyl derivative; R3 is H, alkyl, alkdiyl-OH, alkdiyl-O-alkyl, or alk(en/yn)diyl-C(O)-NH2, etc.; R4 is CO2H, halogen, CN, or OH, etc.; R5 is H, CO2H, CN, halogen, or OP(:O)(OH)2, etc.], useful for treating cellular proliferative diseases, for treating disorders associated with KSP kinesin activity, and for inhibiting KSP kinesin. The invention is also related to compns. which comprise these compds., and methods of using them to treat cancer in mammals. For instance, pyrrolecarboxamide derivative II (kinesin ATPase in vitro assay: IC50 < 50 μM) was prepared via amidation of carbamoyl chloride III by amine IV (conversion of III to the product was >98%).

IT 635724-48-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrolecarboxamide derivs. useful as mitotic kinesin inhibitors)
RN 635724-48-0 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

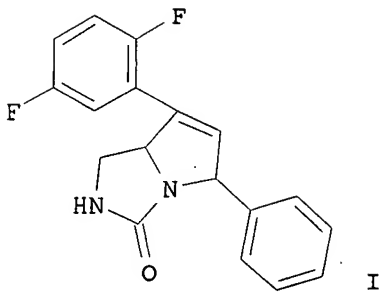
Absolute stereochemistry.



L9 ANSWER 11 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:1156433 CAPLUS
DN 142:69166
TI Bicyclic dihydropyrrole compound mitotic kinesin inhibitors, and therapeutic use
IN Coleman, Paul J.; Neilson, Lou Anne
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004112699	A2	20041229	WO 2004-US18137	20040608
	WO 2004112699	A3	20050414		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004249138	A1	20041229	AU 2004-249138	20040608
	CA 2527533	A1	20041229	CA 2004-2527533	20040608
	EP 1635641	A2	20060322	EP 2004-776354	20040608
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	CN 1805686	A	20060719	CN 2004-80016445	20040608
	JP 2007501863	T	20070201	JP 2006-533604	20040608
	US 2006142278	A1	20060629	US 2005-559855	20051207
PRAI	US 2003-477975P	P	20030612		
	WO 2004-US18137	W	20040608		

OS MARPAT 142:69166
GI



I

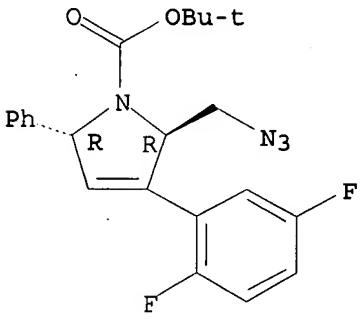
AB The invention discloses bicyclic dihydropyrrole compds. that are useful for treating cellular proliferative diseases, for treating disorders associated with KSP kinesin activity, and for inhibiting KSP kinesin. The invention also discloses compns. which comprise these compds., and methods of using them to treat cancer in mammals. Preparation of compds., e.g. I, is described.

IT 812631-76-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(bicyclic dihydropyrrole compound mitotic kinesin inhibitors, and therapeutic use)

RN 812631-76-8 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 2-(azidomethyl)-3-(2,5-difluorophenyl)-2,5-dihydro-5-phenyl-, 1,1-dimethylethyl ester, (2R,5R)-rel- (9CI) (CA INDEX NAME)

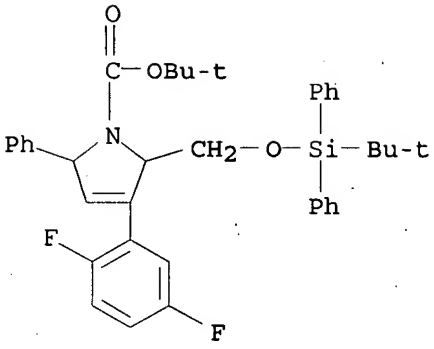
Relative stereochemistry.



IT 812631-69-9P 812631-70-2P 812631-71-3P
812631-72-4P 812631-73-5P 812631-74-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(bicyclic dihydropyrrole compound mitotic kinesin inhibitors, and therapeutic use)

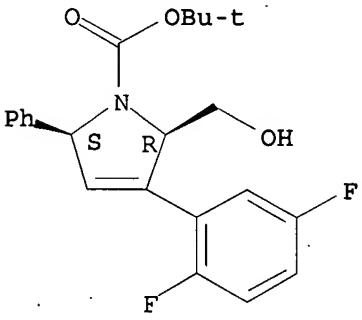
RN 812631-69-9 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 3-(2,5-difluorophenyl)-2-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2,5-dihydro-5-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



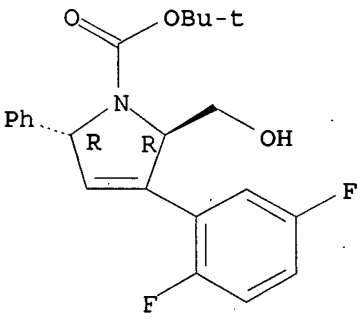
RN 812631-70-2 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 3-(2,5-difluorophenyl)-2,5-dihydro-2-(hydroxymethyl)-5-phenyl-, 1,1-dimethylethyl ester, (2R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



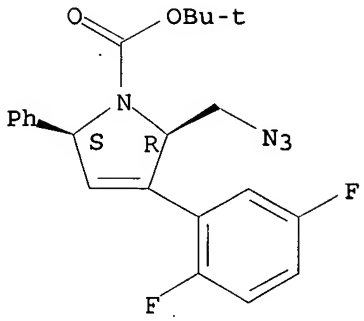
RN 812631-71-3 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 3-(2,5-difluorophenyl)-2,5-dihydro-2-(hydroxymethyl)-5-phenyl-, 1,1-dimethylethyl ester, (2R,5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



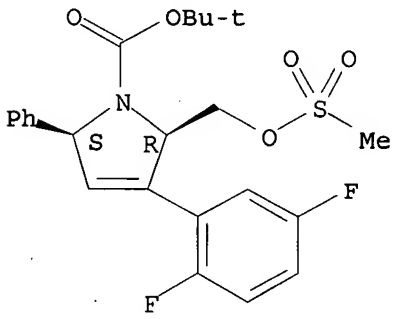
RN 812631-72-4 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-(azidomethyl)-3-(2,5-difluorophenyl)-2,5-dihydro-5-phenyl-, 1,1-dimethylethyl ester, (2R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



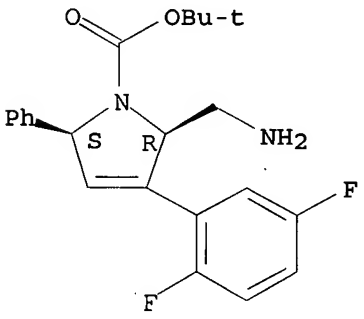
RN 812631-73-5 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 3-(2,5-difluorophenyl)-2,5-dihydro-2-[[(methylsulfonyl)oxy]methyl]-5-phenyl-, 1,1-dimethylethyl ester, (2R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 812631-74-6 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-(aminomethyl)-3-(2,5-difluorophenyl)-2,5-dihydro-5-phenyl-, 1,1-dimethylethyl ester, (2R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

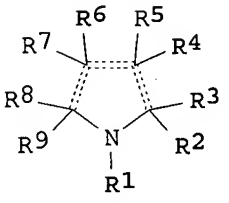


L9 ANSWER 12 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:1127483 CAPLUS
DN 142:74446
TI A preparation of pyrrole derivatives, useful as mitotic kinesin inhibitors
IN Fraley, Mark E.; Garbaccio, Robert M.; Hartman, George D.; Hoffman, William F.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 112 pp.
CODEN: PIXXD2
DT Patent

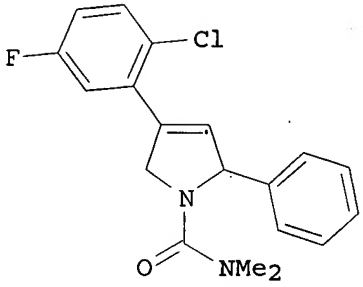
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004111193	A2	20041223	WO 2004-US18065	20040608
	WO 2004111193	A3	20050324		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004248160	A1	20041223	AU 2004-248160	20040608
	CA 2527582	A1	20041223	CA 2004-2527582	20040608
	EP 1636182	A2	20060322	EP 2004-754621	20040608
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	CN 1805928	A	20060719	CN 2004-80016354	20040608
	JP 2007505949	T	20070315	JP 2006-533588	20040608
	US 2006135594	A1	20060622	US 2005-559857	20051207
PRAI	US 2003-477995P	P	20030612		
	WO 2004-US18065	W	20040608		

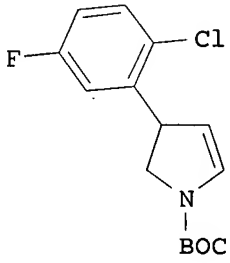
OS MARPAT 142:74446
GI



I



II



III

AB The invention relates to a preparation of pyrrole derivs. of formula I [wherein: R1 is (alkylene)0-1C(O)-alk(en/yn)yl, (alkylene)0-1C(S)-alk(en/yn)yl, or (alkylene)0-1-SO2-alkyl, etc.; R2 and R6 are independently selected from aryl, cycloalkyl, heterocyclyl, or aralkyl; R3, R4, R5, R7, R8, and R9 are independently selected from H, alk(en/yn)yl, aryl, or heterocyclyl, etc.], useful as mitotic kinesin

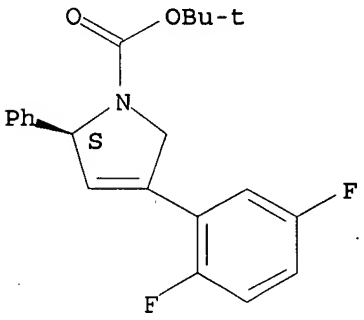
inhibitors (no biol. data). The invention compds. are useful for the treatment of proliferative diseases such as cancer, hyperplasia, restenosis, and immune disorders. For instance, pyrrolecarboxamide derivative II was prepared via phenylation of N-BOC-pyrrol derivative III by PhN2+•BF4-, N-deprotection, and N-carboxamidation by ClC(O)NMe2 (scheme 1).

IT 635724-48-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrrole derivs. useful as mitotic kinesin inhibitors)

RN 635724-48-0 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

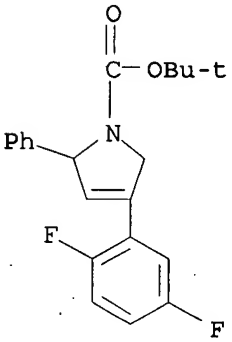
Absolute stereochemistry.



IT 635724-42-4P 639072-35-8P 639074-72-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrole derivs. useful as mitotic kinesin inhibitors)

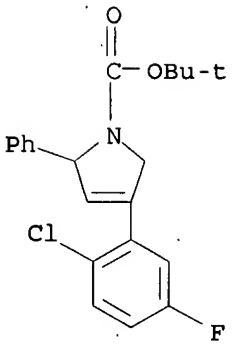
RN 635724-42-4 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

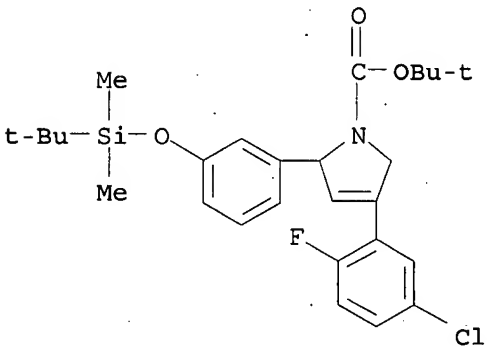


RN 639072-35-8 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2-chloro-5-fluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 639074-72-9 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(5-chloro-2-fluorophenyl)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-2,5-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



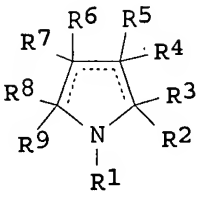
L9 ANSWER 13 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:857324 CAPLUS
DN 141:332040
TI Preparation of dihydropyrrole derivatives as mitotic kinesin inhibitors
IN Slaughter, Donald E.; Subramanian, Raju; Fraley, Mark E.; Prueksaritanont, Thomayant; Shu, Hong
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004087050	A2	20041014	WO 2004-US9027	20040324
	WO 2004087050	A3	20050324		

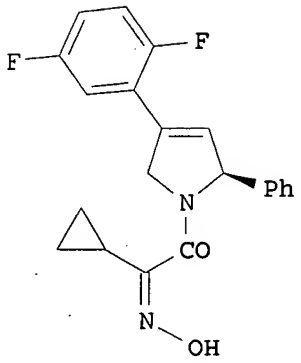
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2003-458494P P 20030328
OS MARPAT 141:332040

GI



I



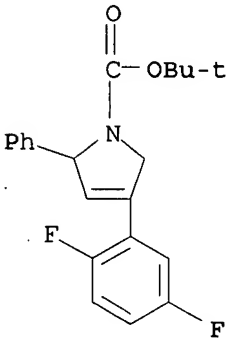
II

AB Dihydropyrrole compds. of formula I [R1 = COCRaNOH, COCRaNO2, etc.; Ra, R2, R6 = aryl, aralkyl, cycloalkyl, heterocyclyl; R3-R5, R7-R9 = H, alkyl, aryl, aralkyl, cycloalkyl, heterocyclyl, etc.] are prepared which are useful for treating cellular proliferative diseases, for treating disorders associated with KSP kinesin activity, and for inhibiting KSP kinesin. The invention also related to compns. which comprise these compds., and methods of using them to treat cancer in mammals. Thus, II was prepared, and had IC50 ≤ 50 μM against kinesin motor domain.

IT 635724-42-4P 635724-48-0P 639072-35-8P
639074-72-9P 639075-47-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dihydropyrrole derivs. as antitumor agents)

RN 635724-42-4 CAPLUS

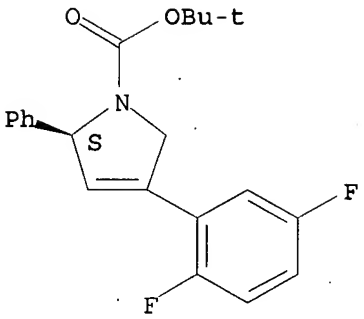
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



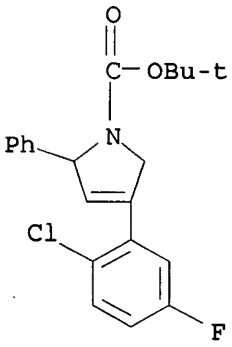
RN 635724-48-0 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

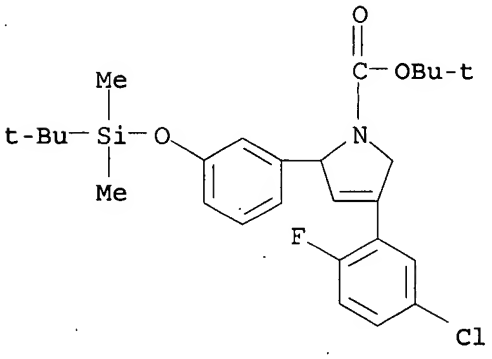
Absolute stereochemistry.



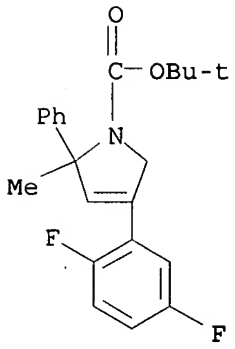
RN 639072-35-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2-chloro-5-fluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 639074-72-9 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(5-chloro-2-fluorophenyl)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-2,5-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



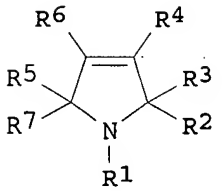
RN 639075-47-1 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-methyl-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



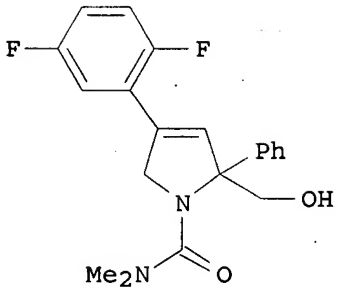
L9 ANSWER 14 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:368866 CAPLUS
DN 140:391193
TI Preparation of dihydropyrroles as mitotic kinesin inhibitors for treating cellular proliferative diseases
IN Breslin, Michael J.; Coleman, Paul J.; Cox, Christopher D.; Hartman, George D.; Mariano, Brenda J.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 178 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004037171	A2	20040506	WO 2003-US32405	20031014
	WO 2004037171	A3	20040708		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2500848	A1	20040506	CA 2003-2500848	20031014
	AU 2003287057	A1	20040513	AU 2003-287057	20031014
	EP 1556052	A2	20050727	EP 2003-777578	20031014
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2006506456	T	20060223	JP 2005-501618	20031014
	US 2006100191	A1	20060511	US 2005-531495	20050415
	US 7235580	B2	20070626		
PRAI	US 2002-419570P	P	20021018		
	US 2003-479712P	P	20030619		
	WO 2003-US32405	W	20031014		

OS MARPAT 140:391193
GI



I



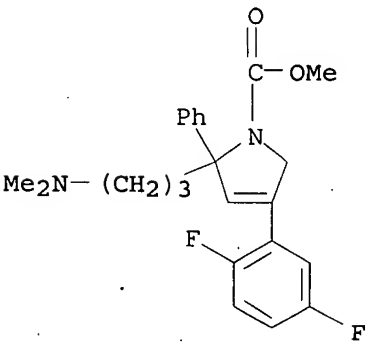
II

AB Title compds. I [wherein R1 = (un)substituted acyl(alkyl), carbamoyl(alkyl), sulfamoyl(alkyl), aryl, heterocyclyl, alkyl, etc.; R2 and R6 = independently (un)substituted aryl(alkyl), cycloalkyl, or heterocyclyl; R3 = (un)substituted alkoxyalk(en/yn)yl, carbamoylalk(en/yn)yl, alkylsulfonylalk(en/yn)yl, etc.; R4, R5, and R7 = independently H or (un)substituted (cyclo)alkyl, alkenyl, alkynyl, perfluoroalkyl, arylalkyl, or heterocyclyl; or R5 and R7 are combined to form an oxo or sulfoxo; or pharmaceutically acceptable salt of stereoisomer thereof] were prepared for treating cellular proliferative diseases, for treating disorders associated with KSP kinesin activity, and for inhibiting KSP kinesin. The invention is also related to compns. which comprise these compds., and methods of using them to treat cancer (no data). For instance, palladium catalyzed Suzuki coupling of 7a-phenyldihydro-1H-pyrrolo[1,2-c][1,3]oxazole-3,6(5H)-dione (multi-step preparation given) and 2,5-difluorophenylboronic acid afforded 6-(2,5-difluorophenyl)-7a-phenyl-5,7a-dihydro-1H-pyrrolo[1,2-c][1,3]oxazol-3-one. The pyrrolooxazolone was treated with NaOH in EtOH to give the (hydroxymethyl)pyrrole, which was O-protected with tert-butyldimethylsilyl chloride. Reaction of the pyrrole with triphosgene and dimethylamine, followed by deprotection using triethylamine trihydrofluoride in MeCN provided II. In a kinesin ATPase assay using a human KSP motor domain construct and microtubules from bovine brain tubulin, example compds. inhibited the ATPase hydrolysis reaction with IC50 ≤ 50 μM.

IT 686321-40-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(KSP inhibitor; preparation of dihydropyrroles as KSP inhibitors for treating proliferative diseases)

RN 686321-40-4 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2-[3-(dimethylamino)propyl]-2,5-dihydro-2-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 15 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN

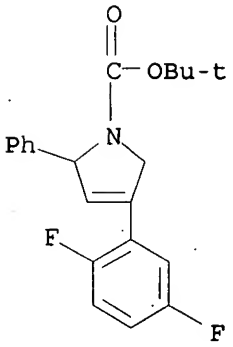
AN 2004:41221 CAPLUS
DN 140:107282
TI Crystal structure of human mitotic kinesin motor domain complexed with ligands and use of the three-dimensional structure in drug discovery
IN Buser-Doepner, Carolyn A.; Coleman, Paul J.; Cox, Christopher D.; Fraley, Mark E.; Garbaccio, Robert M.; Hartman, George D.; Heimbrook, David C.; Kuo, Lawrence C.; Huber, Hans E.; Sardana, Vinod V.; Torrent, Maricel; Yan, Youwei
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 290 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004004652	A2	20040115	WO 2003-US21145	20030703
	WO 2004004652	A3	20041104		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2489562	A1	20040115	CA 2003-2489562	20030703
	AU 2003247891	A1	20040123	AU 2003-247891	20030703
	EP 1551962	A2	20050713	EP 2003-763258	20030703
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005537257	T	20051208	JP 2004-519930	20030703
	US 2006134767	A1	20060622	US 2006-520492	20060130
PRAI	US 2002-394313P	P	20020708		
	WO 2003-US21145	W	20030703		

AB The present invention is directed to the identification, characterization and three-dimensional structure of a novel ligand binding site of kinesin spindle protein (KSP). Binding of ligands to the novel binding site result in a conformational change in the three-dimensional structure of the protein and a modulation of the activity of KSP. This conformational change in turn results in the formation of a novel binding pocket in the KSP protein, which comprises the novel binding site of the instant invention. Compns. and crystals of KSP motor domain with a KSP inhibitor bound to the protein at the novel ligand-binding site are also provided. The crystallized KSP motor domain is phys. analyzed by x-ray diffraction techniques. The resulting x-ray diffraction patterns are of sufficiently high resolution to be useful for determining the three-dimensional structure of inhibitor-bound KSP motor domain. Those atomic coordinates are useful in mol. modeling of related proteins and rational drug design of mimetics and ligands for KSP and related proteins. Methods of using the structure coordinates of KSP motor domain in complex with an inhibitor for the design of pharmaceutical compds. which inhibit the biol. function of KSP, particularly those biol. functions mediated by mol. interactions involving KSP are also disclosed.

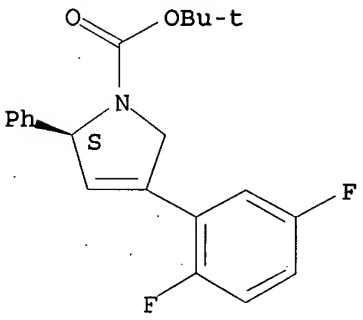
IT 635724-42-4P 635724-48-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of kinesin ligands; crystal structure of human mitotic kinesin motor domain complexed with ligands and use of three-dimensional structure in drug discovery)
RN 635724-42-4 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-

, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 635724-48-0 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



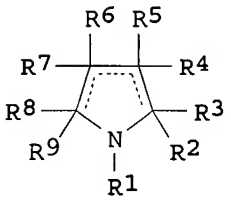
L9 ANSWER 16 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:1006949 CAPLUS
DN 140:42026
TI Preparation of dihydroindolylcarboxylates as mitotic kinesin inhibitors
IN Arrington, Kenneth L.; Fraley, Mark E.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 93 pp.
    CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003106417	A1	20031224	WO 2003-US18694	20030612
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2486215	A1	20031224	CA 2003-2486215	20030612
	AU 2003276005	A1	20031231	AU 2003-276005	20030612
	EP 1515949	A1	20050323	EP 2003-741969	20030612

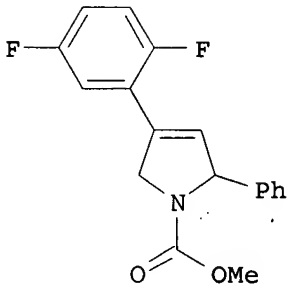
	EP 1515949	B1	20070314		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005533063	T	20051104	JP 2004-513250	20030612
	AT 356804	T	20070415	AT 2003-741969	20030612
	US 2006063942	A1	20060323	US 2004-517576	20041209
PRAI	US 2002-388828P	P	20020614		
	WO 2003-US18694	W	20030612		

OS MARPAT 140:42026

GI



I



II

AB Title compds. I [R1 = carboxy; R2, R6 = aryl, arylalkyl, cycloalkyl, etc.; R3-5, R7-9 = H, alkyl, aryl, alk(en/yn)yl, etc.] are prepared For instance, tert-Bu 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1-carboxylate (preparation given) is coupled to benzenediazonium tetrafluoroborate (CH3CN, Pd2dba3, NaOAc, 23°) to give tert-Bu 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate. This intermediate is deprotected (CH2Cl2, TFA) and converted to II (CH2Cl2, i-Pr2NEt, ClCO2Me). In a kinesin ATPase assay, example compds. exhibit IC50 ≤ 50μM. I are useful for treating cellular proliferative diseases, for treating disorders associated with KSP kinesin activity and for inhibiting KSP kinesin. The invention also related to compns. which comprise these compds. and methods of using them to treat cancer in mammals.

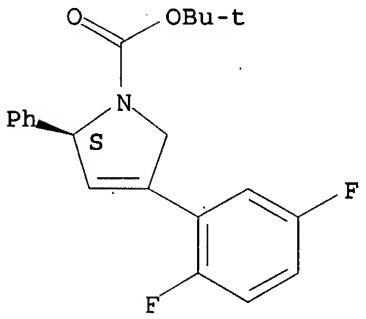
IT 635724-24-2P 635724-25-3P 635724-26-4P
635724-27-5P 635724-28-6P 635724-29-7P
635724-30-0P 635724-31-1P 635724-32-2P
635724-33-3P 635724-34-4P 635724-35-5P
635724-36-6P 635724-37-7P 635724-38-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dihydroindolylcarboxylates as mitotic kinesin inhibitors)

RN 635724-24-2 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, methyl ester (9CI) (CA INDEX NAME)

, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



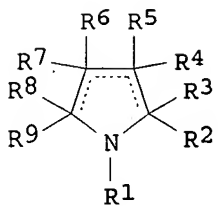
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 17 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:1006780 CAPLUS
DN 140:77020
TI Preparation of pyrrole derivatives as mitotic kinesin inhibitors
IN Arrington, Kenneth L.; Coleman, Paul J.; Cox, Christopher D.; Fraley, Mark E.; Garbaccio, Robert M.; Hartman, George D.; Hoffman, William F.; Tasber, Edward S.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 401 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

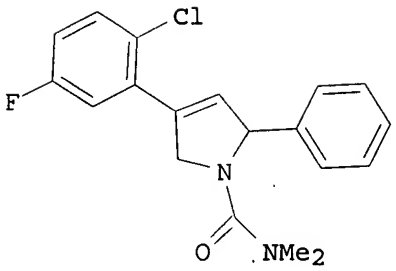
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003105855	A1	20031224	WO 2003-US18482	20030612
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2487489	A1	20031224	CA 2003-2487489	20030612
	AU 2003245453	A1	20031231	AU 2003-245453	20030612
	BR 2003011784	A	20050308	BR 2003-11784	20030612
	EP 1515724	A1	20050323	EP 2003-739093	20030612
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	CN 1674906	A	20050928	CN 2003-819318	20030612
	JP 2005536479	T	20051202	JP 2004-512758	20030612
	ZA 2004009334	A	20060222	ZA 2004-9334	20041119
	US 2006105997	A1	20060518	US 2004-517559	20041208
	IN 2004CN02798	A	20060210	IN 2004-CN2798	20041210
	NO 2005000198	A	20050311	NO 2005-198	20050113
PRAI	US 2002-388621P	P	20020614		
	US 2002-403830P	P	20020815		
	US 2002-426940P	P	20021115		
	US 2003-458318P	P	20030328		
	WO 2003-US18482	W	20030612		

OS MARPAT 140:77020

GI



I



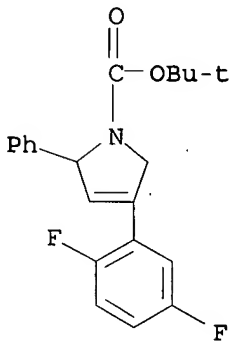
II

AB The invention relates to dihydropyrrole compds. that are useful for treating cellular proliferative diseases and disorders associated with KSP kinesin activity. The invention also relates to compns. which comprise these compds. and methods of using them to treat cancer in mammals. Compds. I [R1 is (C1-C6-alkylene)n-X-R, (n is 0 or 1; X is CO, SO2, NH, PO, etc.; R is alkyl, aryl, amino group, etc.), aryl, heterocyclyl, or alkyl; R2, R6 are aryl, aralkyl, cycloalkyl, or heterocyclyl; R3-R5, R7-R9 are H, alk(en)(yn)yl, aryl, aralkyl, heterocyclyl, etc.] (including amino acid derivs.) are claimed. For example, a detailed synthesis for the preparation of II is outlined, which includes reaction of 2 chloro-5-fluorobenzenediazonium tetrafluoroborate with Boc-protected 2,5-dihydro-1H-pyrrole-1-carboxylate.

IT 635724-42-4P 635724-48-0P 639072-35-8P
639072-50-7P 639074-72-9P 639075-20-0P
639075-47-1P 639075-53-9P 639077-57-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrole derivs. as mitotic kinesin inhibitors)

RN 635724-42-4 CAPLUS

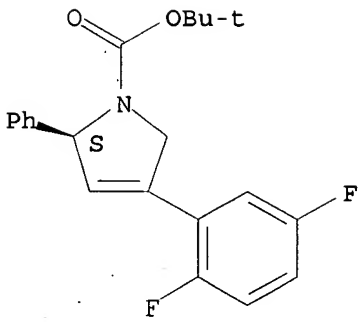
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



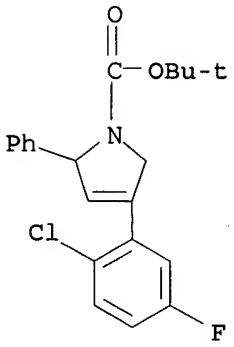
RN 635724-48-0 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

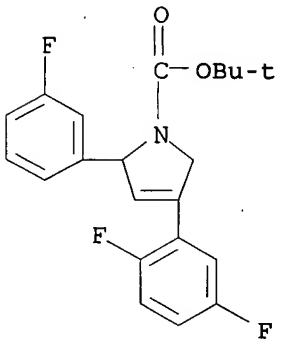
Absolute stereochemistry.



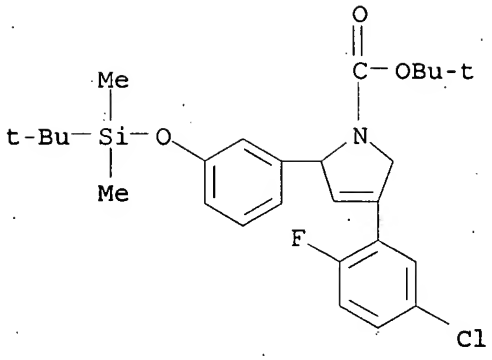
RN 639072-35-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2-chloro-5-fluorophenyl)-2,5-dihydro-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



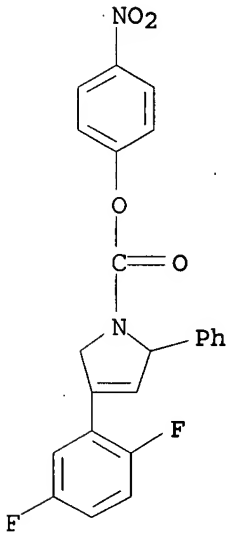
RN 639072-50-7 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2-(3-fluorophenyl)-2,5-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



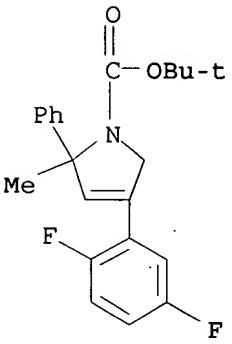
RN 639074-72-9 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(5-chloro-2-fluorophenyl)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-2,5-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 639075-20-0 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

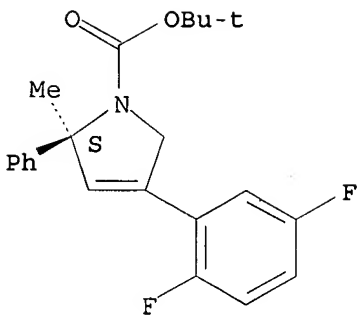


RN 639075-47-1 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-methyl-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

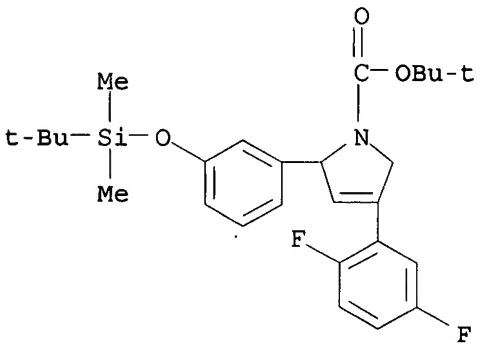


RN 639075-53-9 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2,5-dihydro-2-methyl-2-phenyl-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 639077-57-9 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 4-(2,5-difluorophenyl)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-2,5-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 18 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:396850 CAPLUS
DN 138:401597
TI Preparation of arylpyrrolidinones as neurokinin-1 (NK1) antagonists.
IN Reichard, Gregory A.; Paliwal, Sunil; Shih, Neng-Yang; Xiao, Dong; Tsui, Hon-Chung; Shah, Sapna; Wang, Cheng; Wrobleski, Michelle L.
PA Schering Corporation, USA
SO PCT Int. Appl., 81 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003042173	A1	20030522	WO 2002-US36186	20021112
	WO 2003042173	A8	20031002		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2466465	A1	20030522	CA 2002-2466465	20021112
	AU 2002363642	A1	20030526	AU 2002-363642	20021112

	US 2003144270	A1	20030731	US 2002-292618	20021112
	US 7122677	B2	20061017		
	EP 1451153	A1	20040901	EP 2002-803200	20021112
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	CN 1585748	A	20050223	CN 2002-822380	20021112
	JP 2005509031	T	20050407	JP 2003-544010	20021112
PRAI	US 2001-337652P	P	20011113		
	WO 2002-US36186	W	20021112		

OS MARPAT 138:401597

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

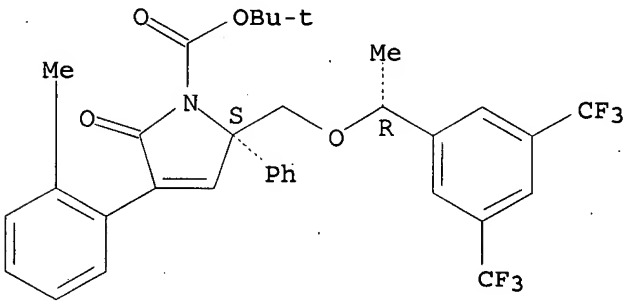
AB Title compds. [I; Q = (CR6R7)n2; X1 = O, S, SO, SO2, NR18a, N(COR12), N(SO2R15); X2 = C, S, SO; Y = O, S, NR11; R1, R2 = H, alkyl, hydroxyalkyl, cycloalkyl, cycloalkylalkyl, CH2F, CHF2 CF3; R1R2 = alkylene, CO; R3 = alkyl, hydroxyalkyl, cycloalkyl, CH2F, CHF2, CF3; R4, R5 = (CR28R29)n1G, C(O)(CR28R29)n4G; n1 = 0-5; n2 = 1-4; n4 = 1-5; G = H, CF3, CHF2, CH2F, OH, alkoxy, SO2R13, cycloalkoxy, NR13R14, SO2NR13R14, NR13SO2R15, NR13COR12NR12(CONR13R14), NR12COC(R12)2NR13R14, CONR13R14, COOR12, cycloalkyl, (R19)r-aryl, (R19)r-heteroaryl, O2CR14, O2CNR13R14, etc.; R4R5 = CO, NR12, atoms to form 4-7 membered ring; R6 = H, alkyl, OR13, SR18; R7 = H, alkyl; R6R7 = CO; R12 = H, alkyl, cycloalkyl, cycloalkylalkyl; R13, R14 = H, alkyl, cycloalkyl, cycloalkylalkyl; R13R14 = atoms to form 4-7 membered ring; R18 = H, alkyl, cycloalkyl, cycloalkylalkyl, P(O)(OH)2; R18a = H, alkyl, cycloalkyl, cycloalkylalkyl; Ar1, Ar2 = (substituted) Ph, heteroaryl; R28, R29 = H, alkyl, CH2F, CHF2, CF3; with provisos], were prepared as NK1 antagonists (no data). Thus, aminoamide (II) was autoclaved with Ba(OH)2 in H2O at 155° followed by treatment (Boc)2O to give 96% Boc-protected acid. The latter in CH2Cl2 was treated with triphosgene and diisopropylethylamine to give 94% cyclic anhydride, which was condensed with EtOAc using LDA in THF to give 88% acetoacetate derivative, which in CH2Cl2 was treated with HCl in dioxane to give title compound (III).

IT 530454-84-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylpyrrolidinones as NK1 antagonists)

RN 530454-84-3 CAPLUS

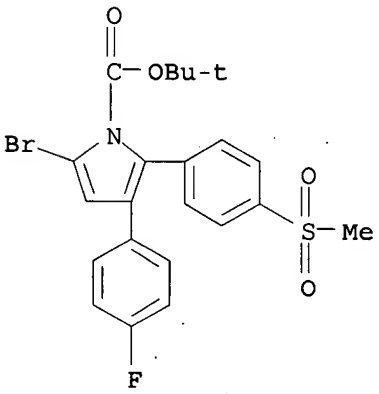
CN 1H-Pyrrole-1-carboxylic acid, 2-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-2,5-dihydro-4-(2-methylphenyl)-5-oxo-2-phenyl-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

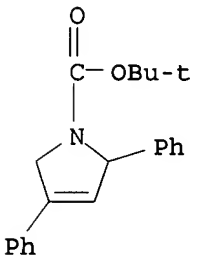
L9 ANSWER 19 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:554334 CAPLUS
DN 133:261093
TI Mechanism of action in a 4,5-diarylpyrrole series of selective cyclo-oxygenase-2 inhibitors
AU Zoete, V.; Maglia, F.; Rougee, M.; Bensasson, R. V.
CS Laboratoire de Chimie Organique Physique, Universite des Sciences et Technologies de Lille, Villeneuve d'Ascq, Fr.
SO Free Radical Biology & Medicine (2000), 28(11), 1638-1641
CODEN: FRBMEH; ISSN: 0891-5849
PB Elsevier Science Inc.
DT Journal
LA English
AB Using semi-empirical AM1 calcn. and 6.31G* basis sets, we have calculated the energy of the highest-occupied MO (EHOMO) for anti-inflammatory 4,5-diarylpyrroles which have been shown to have inhibitory activity on cyclooxygenase COX-2, an inducible enzyme expressed during inflammation. We have found a correlation between the EHOMO of a mol. and its COX-2 inhibition. However, no correlation was observed between EHOMO and the inhibition efficiency of cyclooxygenase-1 (COX-1), the constitutively expressed enzyme, protective to the organism. This result suggests that the inhibitions of the two isoforms follow different mol. mechanisms.
IT 108381-60-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anti-inflammatory mechanism of action of 4,5-diarylpyrroles as selective cyclo-oxygenase-2 inhibitors)
RN 108381-60-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 5-bromo-3-(4-fluorophenyl)-2-[4-(methylsulfonyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

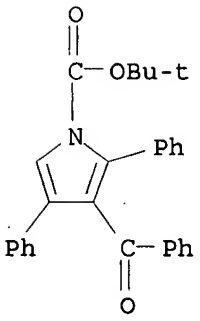
L9 ANSWER 20 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:777606 CAPLUS
DN 132:166085
TI Ring-closing metathesis of phenyl-substituted dienes
AU Bujard, M.; Briot, A.; Gouverneur, V.; Mioskowski, C.
CS Laboratoire de Synthese Bio-Organique, CNRS et Universite Louis Pasteur, Faculte de Pharmacie, Illkirch-Graffenstaden, 67401, Fr.
SO Tetrahedron Letters (1999), 40(50), 8785-8788
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal

LA English
OS CASREACT 132:166085
AB A series of phenyl-substituted heterodienes, CH2:CPhCH2XCRR1CR2:CH2 [X = NHCO2CMe3 with R = R1 = R2 = H, R = Ph, R1 = R2 = H; R = PhCH2, R1 = R2 = H; R = PhCH2O(CH2)5, R1 = R2 = H; R = Me, R1 = Ph, R2 = H; R = R1 = H, R2 = Me or X = O, R = R1 = R2 = H], was prepared and subjected to ring-closure metathesis (RCM) to give differently phenyl-substituted dihydropyrroles and dihydrofuran.
IT 256950-62-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn of hydropyrroles and hydrofuran by ring-closure metathesis of Ph heterodienes)
RN 256950-62-6 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-dihydro-2,4-diphenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

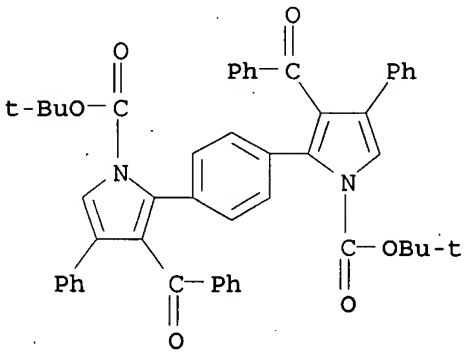


RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

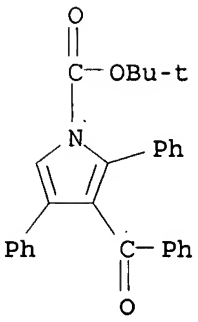
L9 ANSWER 21 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:173742 CAPLUS
DN 131:5312
TI A Direct Synthesis of 2-(Trimethylstannyl)pyrroles from Michael Acceptors and Stannylated Tosylmethyl Isocyanide. [Erratum to document cited in CA129:189411]
AU Dijkstra, Harm P.; ten Have, Ronald; Van Leusen, Albert M.
CS Dep. Organic Molecular Inorganic Chem., Groningen Univ., Groningen, 9747 AG, Neth.
SO Journal of Organic Chemistry (1999), 64(7), 2599
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB The claim that "stannylated pyrroles with a free N-H function have not been reported previously" appears to be incorrect. Two such compds. [5-(tri-n-butylstannyl)pyrrole-2-carbaldehyde (Denat et al., 1992; Veith et al., 1993) and 4-(trimethylstannyl)pyrrole-2-carbaldehyde (Veith et al., 1993)] have been reported by Dubac et al. The latter compds., furthermore, is a second example of a 3-stannylpyrrole.
IT 211741-71-8P 211741-73-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (trimethylstannyl)pyrroles from Michael acceptors and stannylated tosylmethyl isocyanide (Erratum))
RN 211741-71-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 3-benzoyl-2,4-diphenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



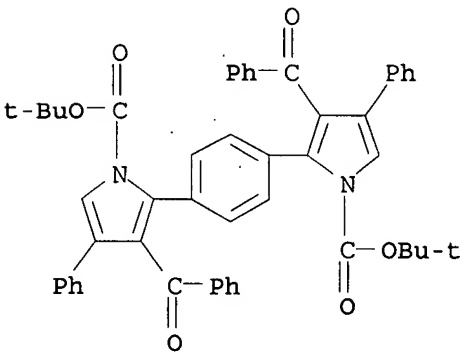
RN 211741-73-0 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,2'-(1,4-phenylene)bis[3-benzoyl-4-phenyl-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



L9 ANSWER 22 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1998:496397 CAPLUS
DN 129:189411
TI A Direct Synthesis of 2-(Trimethylstannyl)pyrroles from Michael Acceptors and Stannylated Tosylmethyl Isocyanide
AU Dijkstra, Harm P.; ten Have, Ronald; van Leusen, Albert M.
CS Department of Organic and Molecular Inorganic Chemistry, Groningen University, Groningen, 9747 AG, Neth.
SO Journal of Organic Chemistry (1998), 63(16), 5332-5338
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB 2-(Trimethylstannyl)pyrroles (3), with substituents at the 3- and 4-positions, were synthesized efficiently by a base-induced reaction of stannylated TosMIC with Michael acceptors. Stille cross-couplings with bromobenzene and double cross-couplings with 1,4-dibromobenzene were achieved successfully with the N-Me derivative and the N-Boc derivative of 3-benzoyl-2-(trimethylstannyl)-4-phenylpyrrole (3a), despite the bulk of these stannylpyrroles. Homo-coupling reactions of the same stannylpyrroles with the corresponding bromopyrroles (prepared from stannylpyrroles 3 and NBS) were unsuccessful, probably for steric reasons.
IT 211741-71-8P 211741-73-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (trimethylstannyl)pyrroles from Michael acceptors and stannylated tosylmethyl isocyanide)
RN 211741-71-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 3-benzoyl-2,4-diphenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 211741-73-0 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,2'-(1,4-phenylene)bis[3-benzoyl-4-phenyl-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 23 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1998:124012 CAPLUS
DN 128:180339
TI Preparation of N-amidinopiperidines and analogs as neuroprotectants
IN Durant, Graham J.; Maillard, Michael; Guo, Jun Qing
PA Cambridge Neuroscience, Inc., USA; Durant, Graham J.; Maillard, Michael; Guo, Jun Qing
SO PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9806401	A1	19980219	WO 1997-US13995	19970808
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 2003069274	A1	20030410	US 1996-694906	19960809
US 6756389	B2	20040629		
CA 2263100	A1	19980219	CA 1997-2263100	19970808
AU 9740577	A	19980306	AU 1997-40577	19970808

	EP 959887	A1	19991201	EP 1997-938194	19970808
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2000516615	T	20001212	JP 1998-509903	19970808
	KR 2000029897	A	20000525	KR 1999-701076	19990209
	AU 766646	B2	20031023	AU 2001-38979	20010427
	US 2005209222	A1	20050922	US 2004-880378	20040628
PRAI	US 1996-694906	A	19960809		
	AU 1997-40577	A3	19970808		
	WO 1997-US13995	W	19970808		

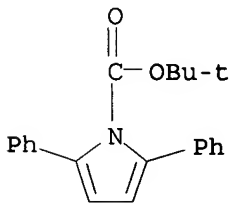
OS MARPAT 128:180339

AB (Un)substituted R1Z1N[C(:NH)NH2]Z2R2 [I; R1R2 = S, O, C, N (sic); Z1 = (CH2)m; Z2 = (CH2)n; m,n = 0-4; m+n ≥ 2] were prepared Thus, 2,6-difluoropyridine was bisarylated by 4-BrC6H4CHMe2 and the product converted in 2 steps to I.HCl [R1R2 = CH2, Z1 = Z2 = 4-(Me2HC)C6H4CHCH2]. Data for biol. activity of I were given.

IT 169782-37-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-amidinopiperidines and analogs as neuroprotectants)

RN 169782-37-0 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 2,5-diphenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 24 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1998:6417 CAPLUS

DN 128:22774

TI Synthesis and (Non)linear Optical Properties of a Series of Donor-Oligopyrrole-Acceptor Molecules

AU Groenendaal, Lambertus; Bruining, Monique J.; Hendrickx, Eric H. J.; Persoons, Andre; Vekemans, Jef A. J. M.; Havinga, Edsko E.; Meijer, E. W.

CS Laboratory of Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.

SO Chemistry of Materials (1998), 10(1), 226-234
CODEN: CMATEX; ISSN: 0897-4756

PB American Chemical Society

DT Journal

LA English

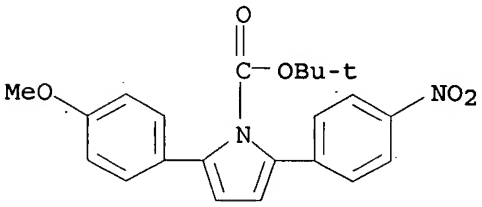
AB The Pd-catalyzed cross-coupling reaction involving organostannanes (Stille reaction) is applied to prepare a series of N-t-BOC-protected D-π-A oligopyrroles. After purification, oligomers with one to four pyrrole units inserted between a 4-nitrophenyl and a 4-methoxyphenyl group are isolated in yields between 20 and 47%. Only minor differences in the linear optical properties are observed for the four oligomers. The charge-transfer band around λmax = 365 nm shows a small, unexpected, hypsochromic shift, while the π-π* band around λmax = 285 nm shows a small, expected, bathochromic shift upon elongation of the mol. Their nonlinear optical properties, however, show a surprising proceeding; going from the D-π-A oligomer with one pyrrole unit to that with three pyrrole units, the hyperpolarizability, as measured by hyper-Rayleigh scattering, increases addnl. with the number of pyrrole units within the

oligomer, up to 277 + 10-30 esu in case of the trimer. On the basis of the assumption that both transitions contribute to the hyperpolarizability, a better conjugated D-π-A oligomer with a bithienyl spacer inserted between a 2-(4-nitrophenyl)-5-pyrrolyl and a 2-(4-methoxyphenyl)-5-pyrrolyl group is prepared analogously. This mol. shows only one combined absorption at λmax = 378 nm for both the charge transfer and the π-π* band, while the hyperpolarizability is as high as 440 + 10-30 esu. These data, showing a very favorable transparency-hyperpolarizability tradeoff, are explained in terms of the contribution of two transitions that are superimposed.

IT 198981-81-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and (non)linear optical properties of donor-oligopyrrole-acceptor mols.)

RN 198981-81-6 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 2-(4-methoxyphenyl)-5-(4-nitrophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 25 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1997:764047 CAPLUS

DN 128:48177

TI Conversion of pyrroles into bi-1,2,5-thiadiazoles: a new route to biheterocycles

AU Duan, Xiao-Guang; Rees, Charles W.

CS Imperial College of Science, Department of Chemistry, Technology and Medicine, London, SW7 2AY, UK

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (21), 3189-3196
CODEN: JCPRB4; ISSN: 0300-922X

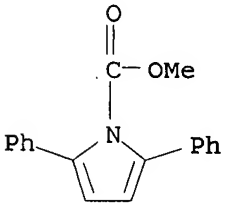
PB Royal Society of Chemistry

DT Journal

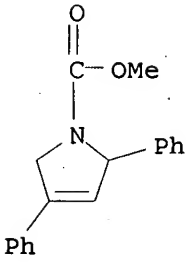
LA English

AB Trithiazyl trichloride (I) converts 1,2,5-triphenylpyrrole (II) into its 3,4-dichloro derivative together with an isothiazole imine (III) and the imine hydrolysis product. The best yield of III is obtained in the presence of 4 Å mol. sieves. Conversion of II into III is exactly analogous to the reaction of I with 2,5-diphenylfuran and -thiophene. Other N-aryl and the related 2,5-diphenylpyrroles give similar results. However, 1-methyl-2,5-diphenylpyrrole reacts with I in an entirely different way to give 4,4'-diphenyl-3,3'-bi-1,2,5-thiadiazole (IV). IV is formed, in similar yields, by reaction of I with 1,4-diphenylbuta-1,3-diyne and 1,4-diphenylbut-1-en-3-yne. Other N-alkyl-2,5-diphenylpyrroles react similarly, giving the best yield (70%) of IV in the presence of 4 Å mol. sieves. 1-Methyl- and 1-ethyl-3,4-dibromo-2,5-diphenylpyrrole also give IV, together with 3-(benzoyldichloromethyl)-4-phenyl-1,2,5-thiadiazole in high combined yield. The formation of IV from N-alkylpyrroles represents a new dissection of the pyrrole ring and a new and very short route to an aromatic biheterocyclic system. Mechanisms which rationalize the different pathways observed are proposed for all of these reactions.

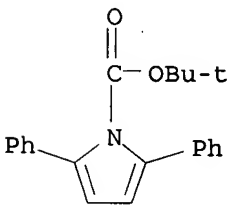
IT 94905-31-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(conversion of pyrroles into bi-1,2,5-thiadiazoles)
RN 94905-31-4 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-diphenyl-, methyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 26 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:367754 CAPLUS
DN 125:86423
TI Regiochemical Control and Suppression of Double Bond Isomerization in the Heck Arylation of 1-(Methoxycarbonyl)-2,5-dihydropyrrole
AU Sonesson, Clas; Larhed, Mats; Nyqvist, Camilla; Hallberg, Anders
CS Department of Pharmacology, Medicinal Chemistry Unit, Goeteborg, S-413 90, Swed.
SO Journal of Organic Chemistry (1996), 61(14), 4756-4763
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 125:86423
AB Arylation of 1-(methoxycarbonyl)-2,5-dihydropyrrole under standard Heck reaction conditions produces a mixture of compds. The olefin undergoes two types of palladium-catalyzed reactions: (a) arylation to provide C-3 arylated derivs. and (b) competing double bond isomerization. Addition of silver carbonate and thallium acetate fully suppressed the isomerization, and good yields of C-3 substituted compds. were achieved after arylation with aryl halides. With regard to aryl triflates as arylating agents, addition of lithium chloride was necessary to promote the Heck reaction. This additive excluded the use of silver and thallium salts, but high regioselectivity and good yields could be obtained by employing tri-2-furylphosphine as ligand. Arylation was rendered both regioselective and enantioselective (58% ee) with 1-naphthyl triflate as substrate utilizing a (R)-BINAP/thallium acetate combination. The C-3 arylated enamides were converted further into the corresponding 3-arylpyrrolidines.
IT 178482-97-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 178482-97-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-dihydro-2,4-diphenyl-, methyl ester (9CI) (CA INDEX NAME)

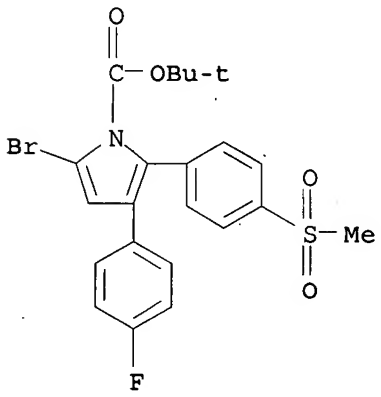


L9 ANSWER 27 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:826853 CAPLUS
DN 123:299788
TI Unusual Redox Behavior of α-Oligoheteroaromatic Compounds: An Increasing First Oxidation Potential with Increasing Conjugation Length
AU van Haare, J. A. E. H.; Groenendaal, L.; Peerlings, H. W. I.; Havinga, E. E.; Vekemans, J. A. J. M.; Janssen, R. A. J.; Meijer, E. W.
CS Laboratory of Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
SO Chemistry of Materials (1995), 7(10), 1984-9
CODEN: CMATEX; ISSN: 0897-4756
PB American Chemical Society
DT Journal
LA English
AB Ph end-capped α-oligoheteroarom. compds. consisting of pyrrole and thiophene units were synthesized via Stille coupling reactions. Cyclic voltammetry studies on diphenyl-α-oligopyrroles (PhPnPh) reveal two chemical reversible oxidation waves for n ≥ 2, with decreasing potentials for larger n. For bis(phenylpyrrolyl)-α-oligothiophenes (PhPTnPPh), in contrast, the authors observe an increase of the 1st and a decrease of the 2nd oxidation potential going from n = 1 to n = 3. The bandgap in both series follows the usual decreasing behavior with increasing conjugation length. The oxidation potentials of both PhPnPh and PhPTnPPh are explained using a Hueckel-type band model. This theor. model indicates that in the oxidized form of PhPTnPPh, the pos. charge tends to localize on the pyrrole units.
IT 169782-37-0P, N-(tert-Butoxycarbonyl)-2,5-diphenylpyrrole
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal removal of N-protecting butoxy group)
RN 169782-37-0 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-diphenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

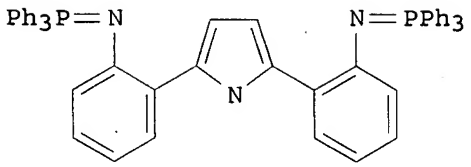


L9 ANSWER 28 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:790898 CAPLUS
DN 123:217724
TI Antiinflammatory 4,5-Diarylpyrroles. 2. Activity as a Function of Cyclooxygenase-2 Inhibition
AU Wilkerson, Wendell Wilkie; Copeland, Robert A.; Covington, Maryanne; Trzaskos, James M.

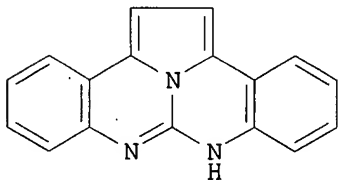
CS DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0353, USA
SO Journal of Medicinal Chemistry (1995), 38(20), 3895-901
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB The antiinflammatory activity of a series of 2-substituted- and 2,3-disubstituted-4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrroles was previously shown by quant. structure-activity relationship (QSAR) studies to be correlated with the molar refractivity and inductive field effect of the 2-substituent and the lipophilicity of the 3-substituent. The present study demonstrates that much of the antiinflammatory activity of these pyrroles could be correlated with the inhibition of the inducible isoform of cyclooxygenase (COX2). Addnl. QSAR studies have been used to identify the mol. parameters necessary for maximizing COX2 inhibition while simultaneously minimizing the inhibition of constitutively expressed cyclooxygenase-1. Such an effort should facilitate the discovery and development of selective COX inhibitors that should lead to safer nonsteroidal antiinflammatory drugs.
IT 108381-60-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antiinflammatory diarylpyrroles: activity as a function of cyclooxygenase-2 inhibition)
RN 108381-60-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 5-bromo-3-(4-fluorophenyl)-2-[4-(methylsulfonyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 29 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:556578 CAPLUS
DN 123:256660
TI Preparation of [5,6,6] tricyclic guanidines from C,C-bis(iminophosphoranes)
AU Molina, Pedro; Alajarin, Mateo; Vidal, Angel
CS Fac. de Quimica, Univ. Murcia, Murcia, E-30071, Spain
SO Tetrahedron (1995), 51(18), 5351-60
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English
OS CASREACT 123:256660
GI



I



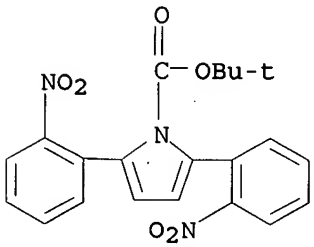
II

AB Aza Wittig-type reaction of N,N'-bis(triphenylphosphoranylidene)-2,2'-(1H-pyrrole-2,5-diyl)bis[benzenamine] (I), the C,C-bis(iminophosphorane) derived from 2,5-bis(o-aminophenyl)pyrrole, with two equivalent of aryl isocyanates gave tricyclic guanidines. These guanidines which underwent elimination of the corresponding diarylcarbodiimide by thermal treatment to give a parent [5,6,6]tricyclic guanidine II.

IT 169139-46-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of tricyclic guanidines from bis(iminophosphoranes))

RN 169139-46-2 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 2,5-bis(2-nitrophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 30 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1994:207906 CAPLUS

DN 120:207906

TI Antiinflammatory 4,5-Diarylpyrroles: Synthesis and QSAR

AU Wilkerson, Wendell W.; Galbraith, William; Gans-Brangs, Kathleen; Grubb, Mary; Hewes, Walter E.; Jaffee, Bruce; Kenney, J. P.; Kerr, Janet; Wong, Nancy

CS DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0353, USA

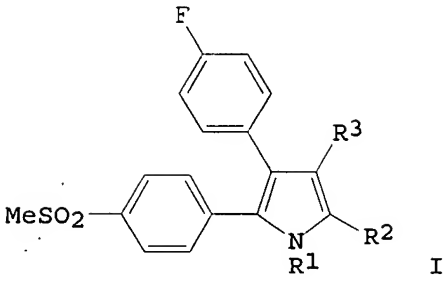
SO Journal of Medicinal Chemistry (1994), 37(7), 988-98
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 120:207906

GI



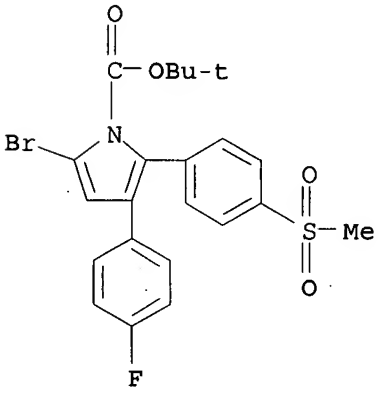
I

AB A series of 2-substituted- and 2,3-disubstituted-4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrroles (I, R1 = e.g., H or Me; R2 = e.g., H halo SCN, SMe, COCF3, NO2, R3 = H or halo) was synthesized and found to be active in the rat adjuvant arthritis model of inflammation. The most active compds. were the 2-halo derivs. in the order of chloro > bromo > iodo. The same pattern of activity was observed for the 2,3-dihalopyrroles. Quant. structure-activity relationship studies suggested that the activity could be correlated with the molar refractivity and the inductive field effect of the 2-substituent and the lipophilicity of the 3-substituent.

IT 108381-60-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anti-inflammatory activity and QSAR of)

RN 108381-60-8 CAPLUS

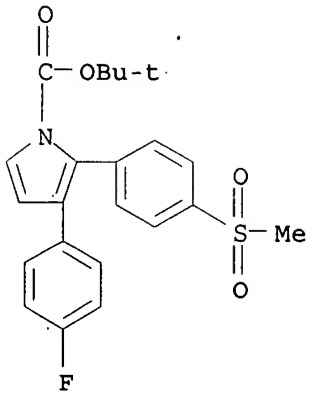
CN 1H-Pyrrole-1-carboxylic acid, 5-bromo-3-(4-fluorophenyl)-2-[4-(methylsulfonyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



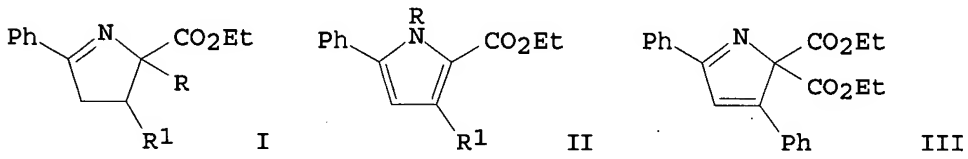
IT 108400-78-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)

RN 108400-78-8 CAPLUS

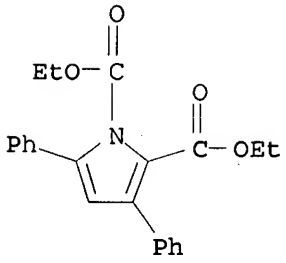
CN 1H-Pyrrole-1-carboxylic acid, 3-(4-fluorophenyl)-2-[4-(methylsulfonyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



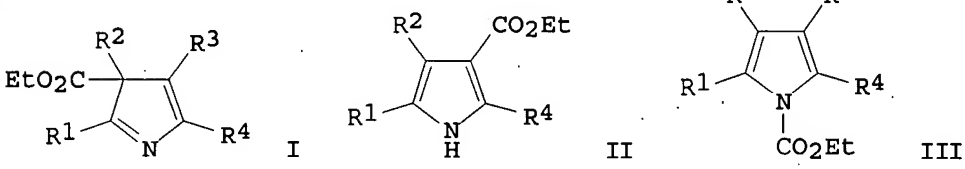
L9 ANSWER 31 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1991:449294 CAPLUS
DN 115:49294
TI Aryl and ethoxycarbonyl derivatives of pyrroles, 2H-pyrroles and 3,4-dihydropyrroles and their immunoactivity on human T lymphocytes
AU Birouk, M.; Harraga, S.; Panouse-Perrin, J.; Robert, J. F.; Damelincourt, M.; Theobald, F.; Mercier, R.; Panouse, J. J.
CS Equipe Chim. Ther., UFR Sci. Med. Pharm., Besancon, 25030, Fr.
SO European Journal of Medicinal Chemistry (1991), 26(1), 91-9
CODEN: EJMCA5; ISSN: 0223-5234
DT Journal
LA French
OS CASREACT 115:49294
GI



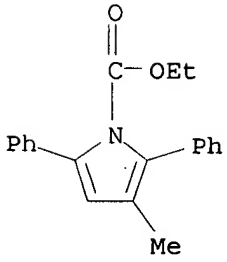
AB Title compds. I (R = CO2Et, R1 = H, Ph; R = H, R1 = Ph), II (R = H, CO2Et, R1 = Ph; R = H, R1 = CO2Et; R = CO2Et, R1 = H), and III were prepared I - III activate human T lymphocytes, II (R = H, R1 = Ph) having better activity than levamisole. A conformational approach based on magnetic anisotropy demonstrates the importance of the orthogonality of the substituent in the 3-position relative to the pyrrole ring for the immunostimulant activity.
IT 91307-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, decarboxylation, and immunostimulant activity of)
RN 91307-93-6 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3,5-diphenyl-, diethyl ester (9CI) (CA INDEX NAME)



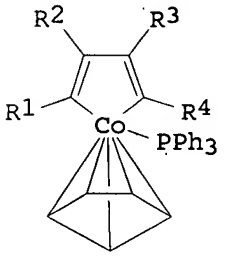
L9 ANSWER 32 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1990:611747 CAPLUS
DN 113:211747
TI The synthesis and chemistry of azolenines. Part 18. Preparation of 3-ethoxycarbonyl-3H-pyrroles via the Paal-Knorr reaction, and sigmatropic rearrangements involving competitive ester migrations to C-2, C-4 and N
AU Chiu, Pak Kan; Sammes, Michael P.
CS Dep. Chem., Univ. Hong Kong, Hong Kong
SO Tetrahedron (1990), 46(10), 3439-56
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
OS CASREACT 113:211747
GI



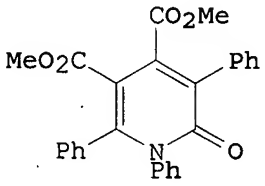
AB 3H-Pyrrole-3-carboxylic esters I [R1 = Me, Ph, CMe, CO2Et; R2 = Me, R3 = H, Me; R4 = Me, Ph, CMe3; R1R2 = (CH2)4, R3 = H, R4 = Me, Ph] were prepared, in some cases together with isomers having exocyclic double bonds, by cyclization. of suitably substituted 2-ethoxycarbonyl-1,4-diketones with liquid ammonia, followed by dehydration of the isolable 2-hydroxy-3,4-dihydro-2H-pyrrole intermediates with aluminia in boiling solvents. Prolonged heating in toluene or p-xylene converts the 3H-pyrroles (I) quant. into isomeric 4-esters II and N-esters III of 1H-pyrroles via competitive [1,5]sigmatropic rearrangements. Isolable intermediate 2H-pyrrole-2-carboxylic esters are converted similarly into the same products, under the same conditions. Detection of 3H-pyrroles as intermediates in the latter reaction demonstrates for the first time the reversibility of the thermal 2H-pyrrole to 3H-pyrrole interconversion.
IT 111400-73-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 111400-73-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 3-methyl-2,5-diphenyl-, ethyl ester (9CI) (CA INDEX NAME)



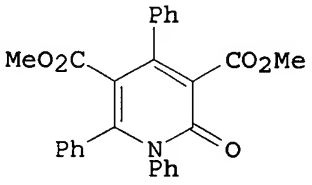
L9 ANSWER 33 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1990:157984 CAPLUS
DN 112:157984
TI Reactions of cobaltacyclopentadiene complexes with organic azides directed toward the synthesis of highly substituted pyrroles
AU Hong, Pangbu; Yamazaki, Hiroshi
CS Inst. Phys. Chem. Res., Wako, 351-01, Japan
SO Journal of Organometallic Chemistry (1989), 373(1), 133-42
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA English
OS CASREACT 112:157984
GI



I



VI



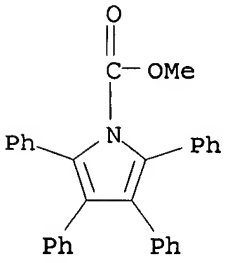
VII

AB The reactions of the cobaltacyclopentadiene complexes I [R1 = R2 = R3 = R4 = Ph (II); R1 = R4 = Ph, R2 = R3 = Me, CO2Me; R1 = R3 = Ph, R2 = R4 = CO2Me (III)] with organic azides were investigated. II reacts with Ph azide at 80° to give 1,2,3,4,5-pentaphenylpyrrole in 73% yield. Similarly, the reactions of II with benzoyl and tert-butoxycarbonyl azides give 1-benzoyl- and 1-(tert-butoxycarbonyl)-2,3,4,5-tetraphenylpyrroles in 41 and 64% yields, resp., but reaction with p-toluenesulfonyl azide gives 2,3,4,5-tetraphenylpyrrole and 3,4,5,6-tetraphenylpyridazine in 35 and 45% yields, resp., in place of the expected 1-(p-toluenesulfonyl)-2,3,4,5-tetraphenylpyrrole. The reaction of I (R1 = R4 = Ph, R2 = R3 = CO2CH3) (IV) with Ph azide at 130° gives 1,2,5-triphenyl-3,4-bis(methoxycarbonyl)pyrrole and 2,5-diphenyl-3,4-bis(methoxycarbonyl)pyrrole (V) in 22 and 15% yields, resp. The reaction of IV with benzenesulfonyl azide gives only V in 57% yield. In the reaction of III with benzenesulfonyl azide, V was unexpectedly obtained in 26% yield, together with 2,4-diphenyl-3,5-bis(methoxycarbonyl)pyrrole (30%), which suggests that a skeletal rearrangement of the metallacycle

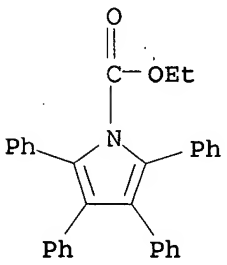
occurs during the reaction. The reaction of IV or III with benzoyl azide at 130° gives the 2(1H)-pyridinone derivs. VI (82%) and VII (53%), which are the products of the reaction of the corresponding cobaltacyclopentadiene with Ph isocyanate generated by the rearrangement of benzoyl nitrene, in place of the expected, corresponding pyrrole.

IT 126087-06-7P 126087-07-8P 126087-08-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

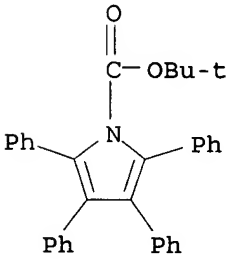
RN 126087-06-7 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,3,4,5-tetraphenyl-, methyl ester (9CI) (CA INDEX NAME)



RN 126087-07-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,3,4,5-tetraphenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 126087-08-9 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,3,4,5-tetraphenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

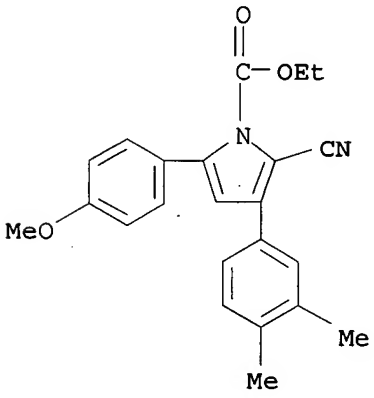


L9 ANSWER 34 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1988:94353 CAPLUS
DN 108:94353
TI The synthesis and chemistry of azolenines. Part 10. Reinvestigation of a reaction reported to yield ethyl 2-cyano-3-(3,4-dimethylphenyl)-5-(4-methoxyphenyl)-2H-pyrrole-2-carboxylate, and thermal rearrangements of this and a regioisomer

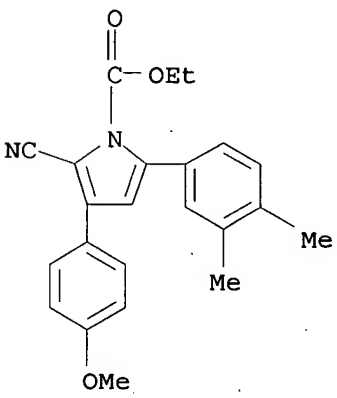
AU Ip, Shing Hong; Sammes, Michael P.
CS Dep. Chem., Univ. Hong Kong, Hong Kong, Hong Kong
SO Journal of Chemical Research, Synopses (1987), (10), 330-1
CODEN: JRPSDC; ISSN: 0308-2342
DT Journal
LA English
OS CASREACT 108:94353
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

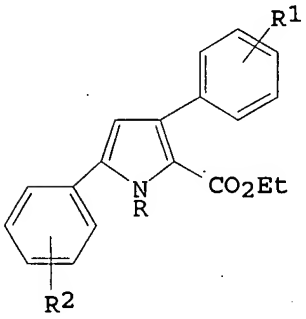
AB Reaction of chalcone I with NCCH2CO2Et and NH4OAc gave pyridines II and III, not pyrrolecarboxylate IV (Moussa, H. H.; Chabaka, L. M., 1983). Thermal rearrangement of IV gave pyrroles V (R = CO2Et, R1 = H; R = H, R1 = CO2Et).
IT 113019-48-0P 113019-50-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 113019-48-0 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-cyano-3-(3,4-dimethylphenyl)-5-(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 113019-50-4 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-cyano-5-(3,4-dimethylphenyl)-3-(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

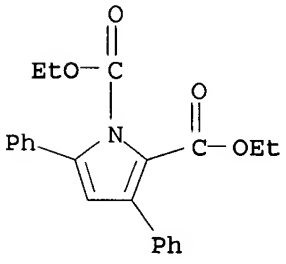


L9 ANSWER 35 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1988:74692 CAPLUS
DN 108:74692
TI The synthesis and chemistry of azolenines. Part 7. Carbon-13 NMR spectra of 3,5-diaryl-1H-pyrrole-2-carboxylic esters, and -1,2-dicarboxylic esters. Complete assignments and substituent chemical shift effects of 3- and 5-aryl ring substituents
AU Chung, Margaret W. L.; Sammes, Michael P.
CS Dep. Chem., Univ. Hong Kong, Hong Kong
SO Journal of Chemical Research, Synopses (1987), (9), 292-3
CODEN: JRPSDC; ISSN: 0308-2342
DT Journal
LA English
GI

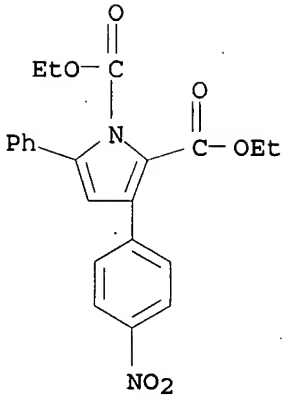


I

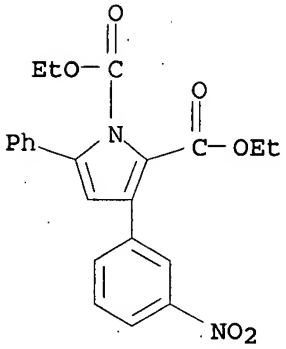
AB Diarylpyrrolecarboxylates I (R = H, CO2Et; R1, R2 = H, 3-NO2, 4-NO2, 4-Cl, 4-Me, 4-MeO) were prepared and their carbon-13 NMR chemical shifts were assigned. Substituent effects of ring substituents on chemical shifts were studied by using Hammett correlations.
IT 91307-93-6 100784-78-9 100784-79-0
100784-80-3 100784-81-4 100784-82-5
100784-83-6 100784-84-7 100784-85-8
100784-86-9 112798-46-6 112798-47-7
RL: PRP (Properties)
(carbon-13 NMR of)
RN 91307-93-6 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3,5-diphenyl-, diethyl ester (9CI) (CA INDEX NAME)



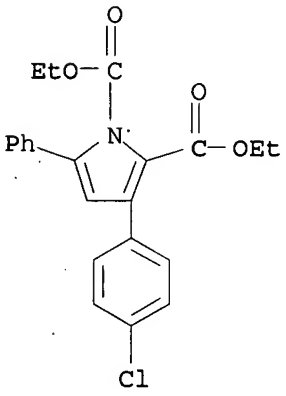
RN 100784-78-9 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(4-nitrophenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



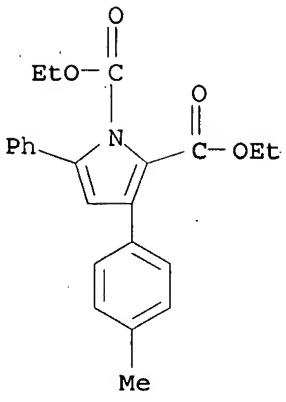
RN 100784-79-0 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(3-nitrophenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



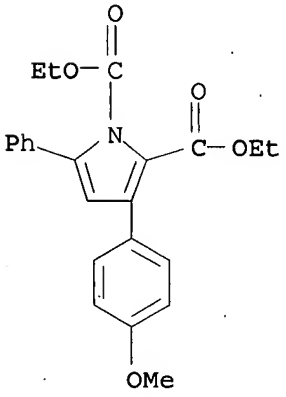
RN 100784-80-3 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(4-chlorophenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



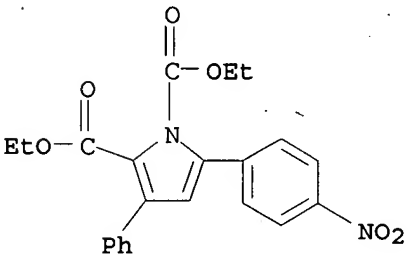
RN 100784-81-4 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(4-methylphenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



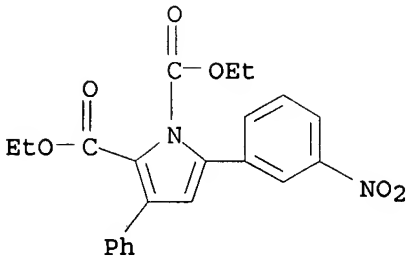
RN 100784-82-5 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(4-methoxyphenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



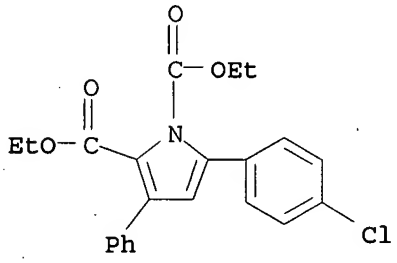
RN 100784-83-6 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 5-(4-nitrophenyl)-3-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



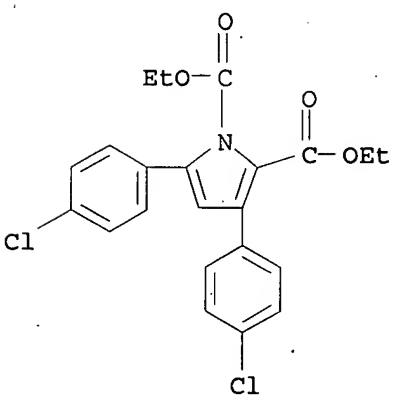
RN 100784-84-7 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 5-(3-nitrophenyl)-3-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



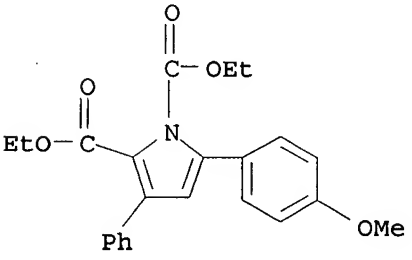
RN 100784-85-8 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 5-(4-chlorophenyl)-3-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



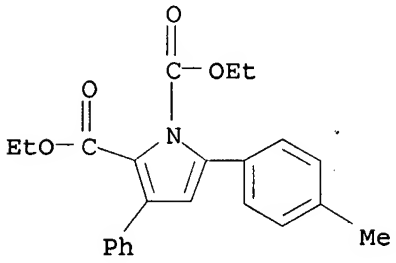
RN 100784-86-9 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3,5-bis(4-chlorophenyl)-, diethyl ester (9CI) (CA INDEX NAME)



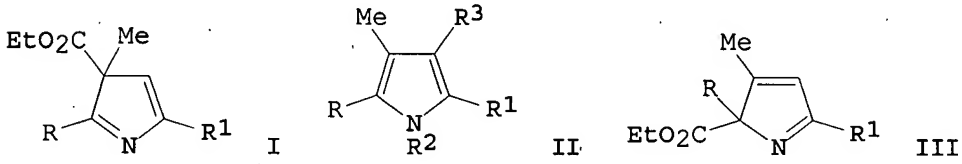
RN 112798-46-6 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 5-(4-methoxyphenyl)-3-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



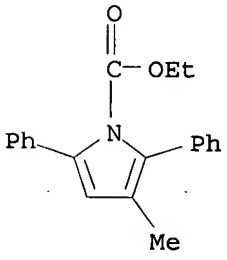
RN 112798-47-7 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 5-(4-methylphenyl)-3-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 36 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1987:636423 CAPLUS
DN 107:236423
TI Thermal rearrangement of 3H-pyrroles by competitive [1,5]-sigmatropic shifts, and the reversibility of the 3H- to 2H-pyrrole interconversion
AU Chiu, Pak Kan; Sammes, Michael P.
CS Dep. Chem., Univ. Hong Kong, Hong Kong, Hong Kong
SO Tetrahedron Letters (1987), 28(24), 2775-8
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 107:236423
GI



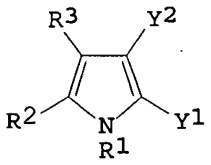
AB 3-Ethoxycarbonyl-3H-pyrroles I (R, R1 = Me, Ph) are converted via thermal [1,5]-ester shifts to the isomeric 1H-pyrrole-4- and N-esters II (R2 = H, R3 = CO2Et; R2 = CO2Et, R3 = H). Isolable intermediate 2H-pyrroles III are converted into the same products, and also into the 3H-pyrroles, demonstrating conclusively the reversibility of the 3H- to 2H-pyrrole interconversion.
IT 111400-73-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 111400-73-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 3-methyl-2,5-diphenyl-, ethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 37 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1987:213759 CAPLUS
DN 106:213759
TI Preparation and formulation of antiinflammatory 2-halo-4,5-diarylpyrroles
IN Wilkerson, Wendell W.
PA du Pont de Nemours, E. I., and Co., USA
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4652582	A	19870324	US 1985-690091	19850109
PRAI US 1985-690091		19850109		

OS CASREACT 106:213759; MARPAT 106:213759
GI

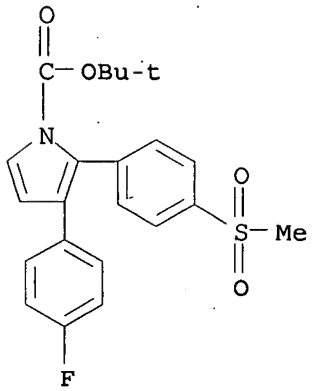


I

AB Title compds. I (R1 = H, Me, Et, Ac, R4O2C, R4 = Me, Et, Me3C, PhCH2; R2, R3 = pyridyl, (un)substituted Ph; Y1 = halo; Y2 = H, Br, Cl) and their salts were prepared by 6 methods. Intermediates for I were also prepared. I (R1, R2, R3 = H; Y1 = 4-MeSO2C6H4; Y2 = 4-FC6H4) in DMF was treated with N-chlorosuccinimide in DMF to give I (R1 = H; R2 = 4-FC6H4; R3 = 4-MeSO2C6H4; Y1 = Cl; Y2 = H) (II). II inhibited adjuvant-induced arthritis in rats with an ED50 of 0.5 mg/kg compared to 305 mg/kg for aspirin. Formulations of I are given.

IT 108400-78-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)

RN 108400-78-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 3-(4-fluorophenyl)-2-[4-(methylsulfonyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

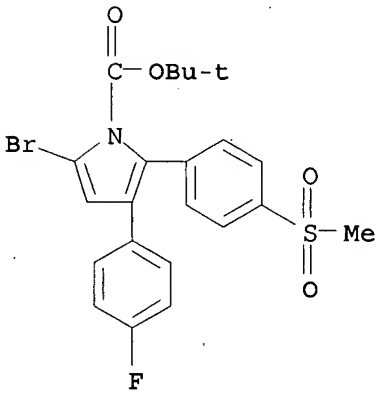


IT 108381-60-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antiinflammatory agent)

RN 108381-60-8 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 5-bromo-3-(4-fluorophenyl)-2-[4-(methylsulfonyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 38 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1986:109402 CAPLUS

DN 104:109402

TI The synthesis and chemistry of azolenines. Part 4. Preparation and rearrangement of some 3,5-diaryl-2H-pyrrole-2,2-dicarboxylic esters

AU Sammes, Michael P.; Chung, Margaret W. L.; Katritzky, Alan R.

CS Dep. Chem., Univ. Hong Kong, Hong Kong, Hong Kong

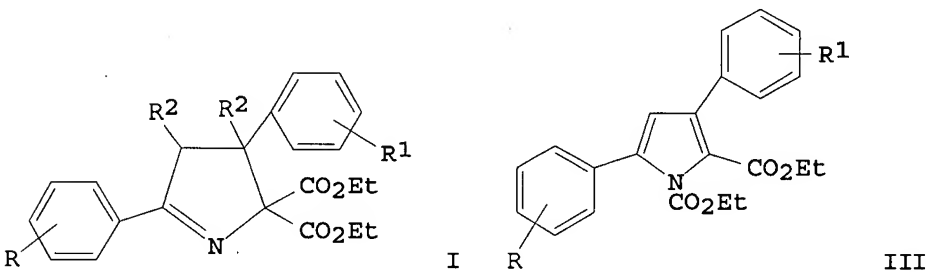
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (8), 1773-9
CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

OS CASREACT 104:109402

GI



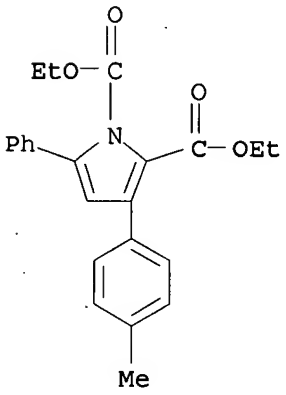
I III

AB Oxidation of dihydropyrroles I (R = H, R1 = H, 4-NO2, 3-NO2, 4-Cl, 4-Me, 4-OMe; R = 4-NO2, 3-NO2, 4-Cl, R1 = H; R = R1 = 4-Cl; R2 = H) (II) with chloranil in refluxing xylene gave the rearranged products III (R, R1 as before) in 58-85% yield and not I (R, R1 as before, R22 = bond) (IV) as previously reported (Robert, J.F.; et al., 1978). IV were obtained from II in 58-82% yield on treatment with DDQ in C6H6 at room temperature IV rearranged to III in refluxing xylene by an acyl [1,5]-sigmatropic shift from C to N, a novel process in 2H-pyrroles. The rearrangement is concerted, with negligible charge separation in the transition state.

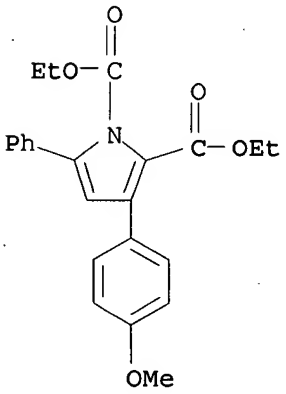
IT 100784-81-4P 100784-82-5P 100784-85-8P

100784-86-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)

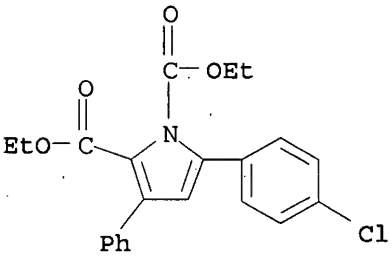
RN 100784-81-4 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(4-methylphenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



RN 100784-82-5 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(4-methoxyphenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)

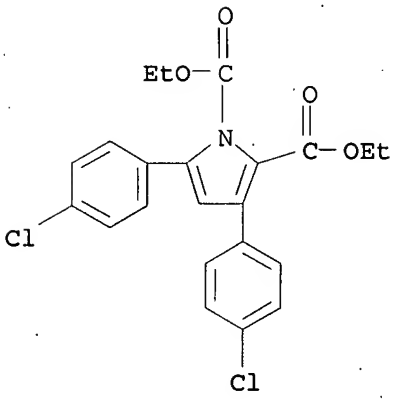


RN 100784-85-8 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 5-(4-chlorophenyl)-3-phenyl-, diethyl ester (9CI) (CA INDEX NAME)

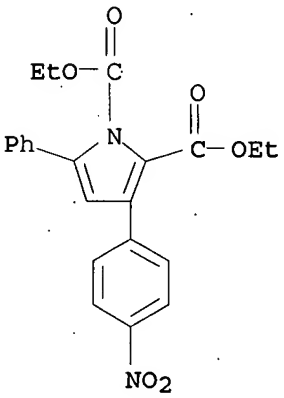


RN 100784-86-9 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3,5-bis(4-chlorophenyl)-, diethyl ester

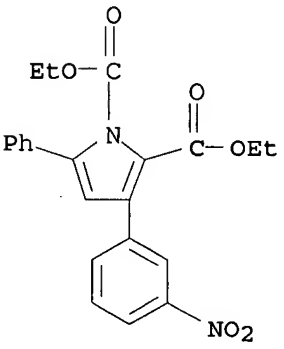
(9CI) (CA INDEX NAME)



IT 100784-78-9P 100784-79-0P 100784-80-3P
100784-83-6P 100784-84-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 100784-78-9 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(4-nitrophenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)

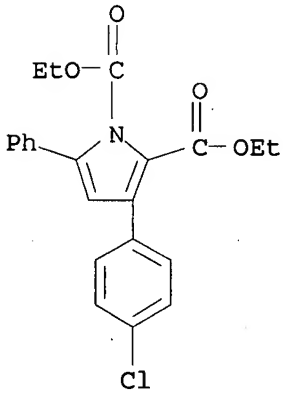


RN 100784-79-0 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(3-nitrophenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)

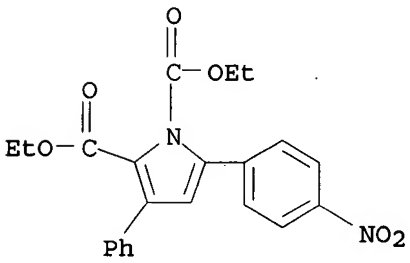


RN 100784-80-3 CAPLUS

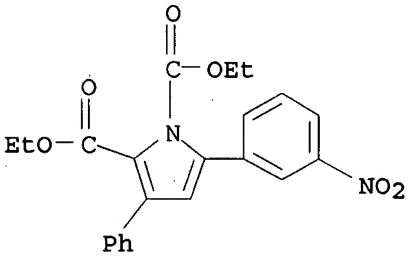
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(4-chlorophenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



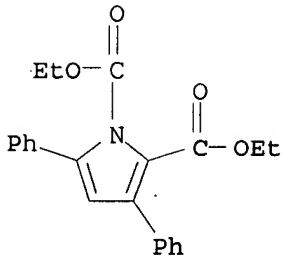
RN 100784-83-6 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 5-(4-nitrophenyl)-3-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



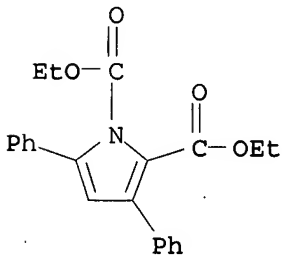
RN 100784-84-7 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 5-(3-nitrophenyl)-3-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



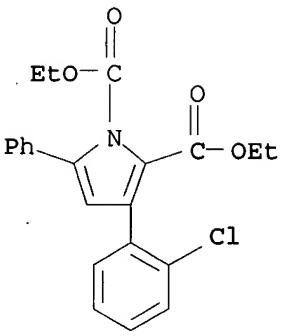
IT 91307-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, decarboxylation, and hydrolysis of)
RN 91307-93-6 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3,5-diphenyl-, diethyl ester (9CI) (CA INDEX NAME)



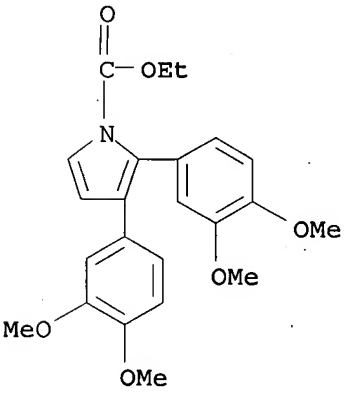
L9 ANSWER 39 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1984:482038 CAPLUS
DN 101:82038
TI Compared structures of two pyrroles: diethyl 3,5-diphenylpyrrole-1,2-dicarboxylate, C22H21NO4 (1), and diethyl 3-(2-chlorophenyl)-5-phenylpyrrole-1,2-dicarboxylate, C22H20ClNO4 (2)
AU Laarif, Ahmed; Theobald, Francois; Birouk, Mohamed; Robert, Jean Francois
CS Lab. Chim. Gen., UER Sci. Exactes Nat., Besancon, 25030, Fr.
SO Acta Crystallographica, Section C: Crystal Structure Communications (1984), C40(7), 1278-81
CODEN: ACSCEE; ISSN: 0108-2701
DT Journal
LA French
AB Title compound 1 is orthorhombic, space group Pbca, with a 17.213(3), b 18.910(3), and c 11.968(3) Å; Z = 8 for dc = 1.239; Rw = 0.081 for 1762 reflections. Title compound 2 is also orthorhombic, space group Pbca, with a 16.955(3), b 18.487(4), and c 13.048(2) Å, Z = 8 for dc = 1.293. Rw = 0.067 For 3122 reflections. The modifications of the angles between the Ph groups and the pyrrole ring agree with the magnetic nonequivalence of the ethoxycarbonyl chains, which is more pronounced in 2. The 3 aromatic rings are planar. The carbonyl groups are planar: that attached to C(2) is coplanar with the pyrrole ring plane, but that attached to N is inclined to the ring plane by 72.4(7)° for 1 and 67.0(4)° for 2. Atomic coordinates are given.
IT 91307-93-6 91307-94-7
RL: PRP (Properties)
(structure of)
RN 91307-93-6 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3,5-diphenyl-, diethyl ester (9CI) (CA INDEX NAME)



RN 91307-94-7 CAPLUS
CN 1H-Pyrrole-1,2-dicarboxylic acid, 3-(2-chlorophenyl)-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 40 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1983:522252 CAPLUS
DN 99:122252
TI An efficient synthesis of substituted isoquinolines
AU Hendrickson, James B.; Rodriguez, Cesar
CS Edison Chem. Lab., Brandeis Univ., Waltham, MA, 02254, USA
SO Journal of Organic Chemistry (1983), 48(19), 3344-6
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 99:122252
AB Aromatic aldehydes can be annelated to isoquinolines in three mild reactions in one vessel, without isolation of intermediates, by successive treatment with H2NCH2CH(OMe)2, ClCO2Et, P(OMe)3, and TiCl4.
IT 86712-49-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 86712-49-4 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,3-bis(3,4-dimethoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

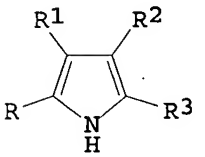


L9 ANSWER 41 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1981:461982 CAPLUS
DN 95:61982
TI Antiinflammatory 4,5-diaryl-2-(substituted-thio)pyrroles and their corresponding sulfoxides and sulfones
IN Cherkofsky, Saul C.
PA du Pont de Nemours, E. I., and Co. , USA
SO U.S., 17 pp. Cont.-in-part of U.S. Ser. No. 10,259, abandoned.
CODEN: USXXAM
DT Patent

LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4267184	A	19810512	US 1980-122501	19800219
	DK 7900757	A	19790914	DK 1979-757	19790221
	NO 7900821	A	19790914	NO 1979-821	19790312
	ES 478556	A1	19791216	ES 1979-478556	19790312
	ZA 7901150	A	19800326	ZA 1979-1150	19790312
	CA 1126275	A1	19820622	CA 1979-323172	19790312
	SU 1005657	A3	19830315	SU 1979-2734803	19790312
	FI 7900852	A	19790914	FI 1979-852	19790313
	AU 7945040	A	19790920	AU 1979-45040	19790313
	AU 527243	B2	19830224		
	JP 54141766	A	19791105	JP 1979-29267	19790313
	HU 22715	A2	19820628	HU 1979-DU302	19790313
	HU 180223	B	19830228		
	ES 484196	A1	19800516	ES 1979-484196	19790914
	DK 8004484	A	19810820	DK 1980-4484	19801023
	AU 8064032	A	19810827	AU 1980-64032	19801031
	AU 540613	B2	19841129		
	IL 61768	A	19840430	IL 1980-61768	19801219
	FI 8004028	A	19810820	FI 1980-4028	19801223
	ZA 8008109	A	19820728	ZA 1980-8109	19801230
	JP 56150060	A	19811120	JP 1981-1642	19810110
	JP 02050902	B	19901105		
	CA 1144550	A1	19830412	CA 1981-369095	19810122
	EP 34798	A2	19810902	EP 1981-101133	19810217
	EP 34798	A3	19810909		
	EP 34798	B1	19850522		
	R: BE, CH, DE, FR, GB, IT, LU, NL, SE				
	NO 8100547	A	19810820	NO 1981-547	19810218
	ES 499559	A2	19830101	ES 1981-499559	19810218
	AT 8100739	A	19831015	AT 1981-739	19810218
	AT 374796	B	19840525		
	SU 1160934	A3	19850607	SU 1981-3248461	19810219
PRAI	US 1978-886337	A2	19780313		
	US 1978-972201	A2	19781228		
	US 1979-10259	A2	19790208		
	IL 1979-56856	A0	19790312		
	US 1980-122501	A	19800219		

OS CASREACT 95:61982; MARPAT 95:61982
GI

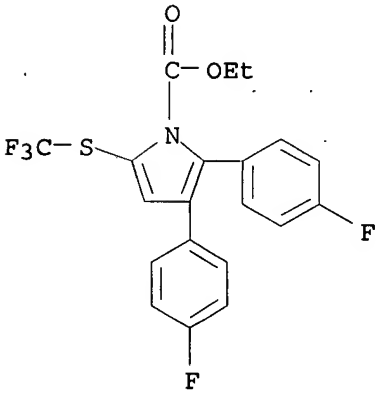


I

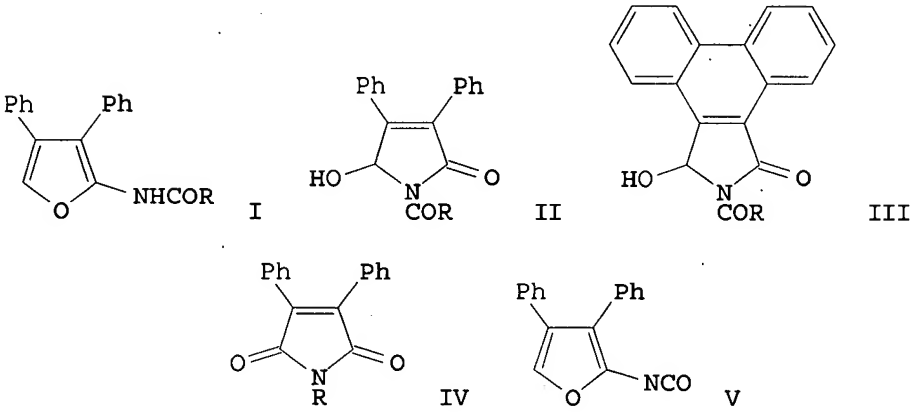
AB About 120 title compds. (I, R, R1 = aryl; R2 = H, alkyl; R3 = H, SCF3, thiocyanato, alkyl- or alkenylthio, alkylsulfonyl or -sulfinyl) were prepared and tested for their antiinflammatory and analgesic activities. Thus, 20 g I (R = R1 = Ph, R2 = R3 = CO2H), obtained by cyclization of PhCOCHPhNH2 with MeO2CC.tplbond.CCO2Me in the presence of NaOAc followed by hydrolysis, was refluxed in quinoline to give 12 g I (R = R1 = Ph, R2 = R3 = H).

IT 73800-58-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antiinflammatory and analgesic activities of)

RN 73800-58-5 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,3-bis(4-fluorophenyl)-5-[(trifluoromethyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)

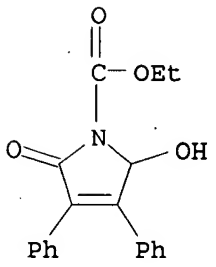


L9 ANSWER 42 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1981:424691 CAPLUS
DN 95:24691
TI Ring transformation of 3,4-diphenyl-2-furylcarbamoyl compounds to N-substituted 3,4-diphenyl-5-hydroxy-3-pyrrolin-2-ones
AU Yakushijin, Kenichi; Kozuka, Masamichi; Furukawa, Hiroshi
CS Fac. Pharm., Meijo Univ., Nagoya, 468, Japan
SO Chemical & Pharmaceutical Bulletin (1980), 28(7), 2178-84
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
OS CASREACT 95:24691
GI

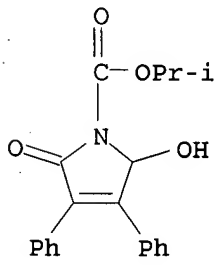


AB Autoxidn. of furans I (R = OCH2Ph, OEt, OCH2Me2, SCH2Ph, NHCH2Ph) gave 21-64% pyrrolinones II, photocyclization of which gave 55-70% phenanthropyrrolinones III. Pyrrolinones II (R = NHCH2Ph, NHPr, NHCHMe2, NHCH2CHMe2) and IV were prepared in 28-33% and 30-4% yield resp. by treating furyl isocyanates V with RNH2.
IT 69018-62-8P 69018-63-9P 69275-55-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)

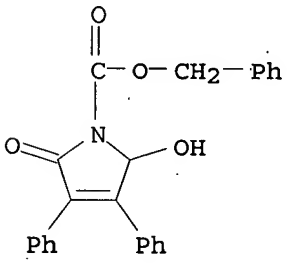
RN 69018-62-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-dihydro-2-hydroxy-5-oxo-3,4-diphenyl-, ethyl ester (9CI) (CA INDEX NAME)



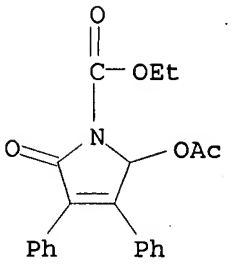
RN 69018-63-9 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-dihydro-2-hydroxy-5-oxo-3,4-diphenyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)



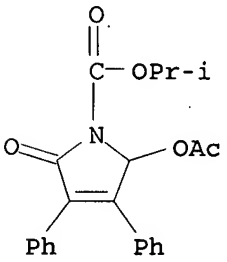
RN 69275-55-4 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-dihydro-2-hydroxy-5-oxo-3,4-diphenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



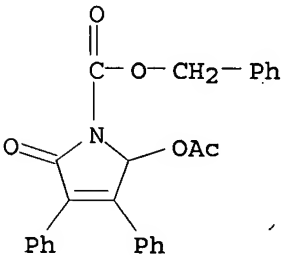
IT 69018-64-0P 69018-65-1P 76394-32-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 69018-64-0 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-(acetyloxy)-2,5-dihydro-5-oxo-3,4-diphenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 69018-65-1 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-(acetyloxy)-2,5-dihydro-5-oxo-3,4-diphenyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 76394-32-6 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-(acetyloxy)-2,5-dihydro-5-oxo-3,4-diphenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



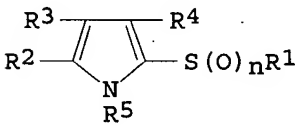
L9 ANSWER 43 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1980:408007 CAPLUS
DN 93:8007
TI 4,5-Diaryl-2-(substituted-thio)-pyrroles and their corresponding sulfoxides and sulfones and pharmaceutical compositions containing them
IN Cherkofsky, Saul Carl
PA du Pont de Nemours, E. I., and Co., USA
SO Eur. Pat. Appl., 52 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 5156	A1	19791114	EP 1979-100736	19790312
	EP 5156	B1	19820922		
	R: BE, CH, DE, FR, GB, IT, LU, NL, SE				
	DK 7900757	A	19790914	DK 1979-757	19790221
	NO 7900821	A	19790914	NO 1979-821	19790312
	ES 478556	A1	19791216	ES 1979-478556	19790312

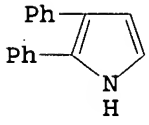
	ZA 7901150	A	19800326	ZA 1979-1150	19790312
	CA 1126275	A1	19820622	CA 1979-323172	19790312
	FI 7900852	A	19790914	FI 1979-852	19790313
	AU 7945040	A	19790920	AU 1979-45040	19790313
	AU 527243	B2	19830224		
	JP 54141766	A	19791105	JP 1979-29267	19790313
	HU 22715	A2	19820628	HU 1979-DU302	19790313
	HU 180223	B	19830228		
	ES 484196	A1	19800516	ES 1979-484196	19790914
PRAI	US 1978-886337		19780313		
	US 1978-972201		19781228		
	US 1979-10259		19790208		

OS MARPAT 93:8007

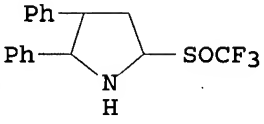
GI



I



II



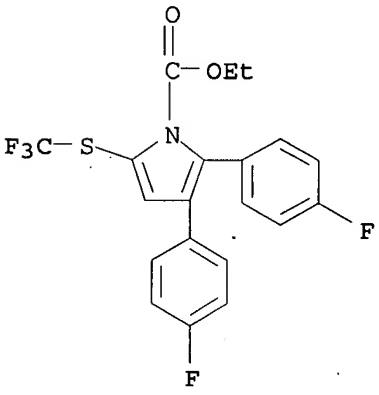
III

AB The title compds. I (R1 = C1-4 alkyl, fluorinated alkyl, allyl; R2, R3 = Ph, substituted Ph, heterocyclyl; R4 = H, C1-3 alkyl; R5 = H, C1-4 alkyl, substituted alkyl, acyl, aroyl, etc.; n = 0, 1, 2), useful as inflammation inhibitors and analgesics (data tabulated for .apprx.65 compds.), were prepared by various methods. Thus, reaction of II with CF3SCl, then oxidation of the resultant sulfide gave III, which has ED50 = 23 mg/kg antiinflammatory and 63 mg/kg analgesic activity with rats.

IT 73800-58-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antiinflammatory and analgesic properties of)

RN 73800-58-5 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 2,3-bis(4-fluorophenyl)-5-[(trifluoromethyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 44 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1979:87178 CAPLUS

DN 90:87178

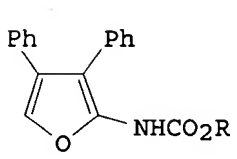
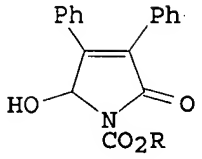
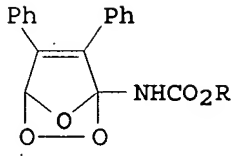
TI A mild autoxidation of 3,4-diphenyl-2-furyl carbamates to 3,4-diphenyl-5-hydroxy-3-pyrrolin-2-ones

AU Ito, Kazuo; Yakushijin, Kenichi

CS Fac. Pharm., Meijo Univ., Nagoya, Japan

SO Heterocycles (1978), 9(11), 1603-6

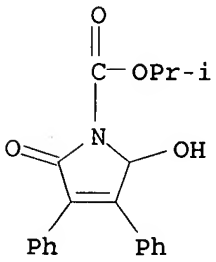
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English
OS CASREACT 90:87178
GI


I

II

III

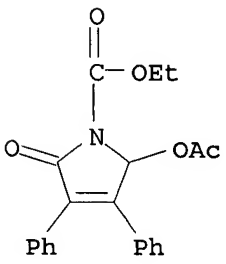
AB Furyl carbamates I (R = benzyl, Et, Me2CH) were treated with O in C6H6 at room temperature to give pyrrolinones II. II (R = Et, Me2CH) were acetylated to give the resp. acetates. Hydrogenolysis of I (R = benzyl) gave 3,4-diphenyl-3-pyrrrolin-2-one. A proposed mechanism for the autoxidn. proceeded through peroxides III and OCHCPh:CPhCONHCO2R as intermediates.

IT 69018-63-9P 69018-64-0P 69018-65-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

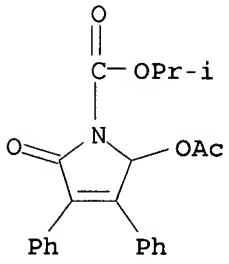
RN 69018-63-9 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-dihydro-2-hydroxy-5-oxo-3,4-diphenyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)



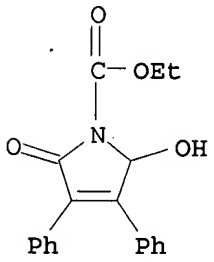
RN 69018-64-0 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-(acetyloxy)-2,5-dihydro-5-oxo-3,4-diphenyl-, ethyl ester (9CI) (CA INDEX NAME)



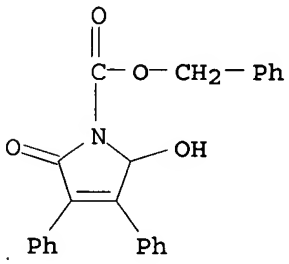
RN 69018-65-1 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2-(acetyloxy)-2,5-dihydro-5-oxo-3,4-diphenyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)



IT 69018-62-8P 69275-55-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by autoxidn. of diphenylfuryl carbamates)
RN 69018-62-8 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-dihydro-2-hydroxy-5-oxo-3,4-diphenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 69275-55-4 CAPLUS
CN 1H-Pyrrole-1-carboxylic acid, 2,5-dihydro-2-hydroxy-5-oxo-3,4-diphenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



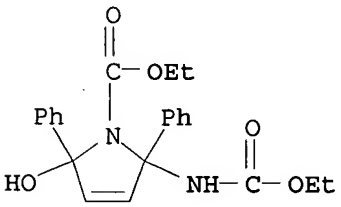
L9 ANSWER 45 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1968:419101 CAPLUS
DN 69:19101
TI Photolysis of a dihydropyridazine. Transformations of the resulting dicarbamate
AU Rigaudy, J.; Breliere, J. C.
CS Ecole Super. Phys. Chim. Ind., Paris, Fr.
SO Bulletin de la Societe Chimique de France (1968), (1), 455-7
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA French
OS CASREACT 69:19101
GI For diagram(s), see printed CA Issue.
AB N,N'-Dicarbethoxy-3,6-diphenyl-1,2-pyridazine was irradiated in Et2O with a high-pressure Hg arc lamp to give 85% EtO2CN:CPhCH:CHCPh:NCO2Et, m. 79-80°. It was hydrolyzed to cis-1,2-dibenzoylethylene, m. 134°, on treatment with 1% H2SO4. It added 1 mol. H2O on treatment

with aqueous HOAc or dioxane to give I, m. 127-8°. This was also hydrolyzed to cis-1,2-dibenzoylethylene. I was catalytically reduced to give the dihydro derivative, which in turn was hydrolyzed to cis-1,2-dibenzoylethane, m. 144°. Reduction of I with LiAlH4 gave N-methyl-2,5-diphenylpyrrole, m. 202°. On treatment with NaOH in Me2CO I gave PhCOCH:CHC(NHCO2Et)2Ph, m. 148°, while its dihydro derivative gave PhCOCH2CH2C(NHCO2Et)2Ph, m. 115-16°. They were hydrolyzed by 1% H2SO4 to give trans-1,2-dibenzoylethylene, m. 110-11°, and 1,2-dibenzoylethane, resp. The compds. were identified by their ir, uv and N.M.R. spectra.

IT 18584-34-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18584-34-4 CAPLUS

CN 3-Pyrroline-2-carbamic acid, 1-carboxy-5-hydroxy-2,5-diphenyl-, diethyl ester (8CI) (CA INDEX NAME)



L9 ANSWER 46 OF 46 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1962:79330 CAPLUS

DN 56:79330

OREF 56:15461b-i

TI Diels-Alder reactions of 1-carbomethoxypyrroles and dimethyl acetylenedicarboxylate

AU Gabel, Norman W.

CS Univ. of Chicago

SO Journal of Organic Chemistry (1962), 27, 301-3
CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

GI For diagram(s), see printed CA Issue.

AB In an attempt to synthesize derivs. of 7-azabicyclo[2.2.1]hepta-2,5-diene, equimolar amts. of I (R1 = R2 = Me) (II) and (.tplbond.CCO2Me)2 (III) were heated to 160° with production of IV (R1 = R2 = Me) (V), by assumed transient formation of the heptadiene adduct and a reverse Diels-Alder reaction. K (0.85 mole) and 0.85 mole 2,5-dimethylpyrrole in 750 ml. dry Et2O stirred vigorously (ice-salt bath) with dropwise addition of 0.86 mole ClCO2Me, the precipitated KCl washed with Et2O, the combined filtrate and washings evaporated, and the residue distilled yielded 59% II, b2 86-90°, m. 38°, λ 250 mμ (ε 5340, MeOH). K (7 g.) and 14.8 g. 2-methylpyrrole in 100 ml. ligroine (b. 90-100°) similarly treated with 19.0 g. ClCO2Me yielded 51% I (R1 = Me, R2 - H), b21 63-5°, n20D 1.493, λ 242, 227 mμ (ε 3640, 7280, MeOH). C4H4NK (from 0.5 mole pyrrole and K) in 500 ml. Et2O treated dropwise with vigorous stirring with 0.52 mole ClCO2Me in 150 ml. Et2O at a rate maintaining gentle refluxing and the filtered solution evaporated yielded 66% I (R1 = R2 = H), b21 71-3°, n20D 1.487, λ 230 mμ (ε 8300, MeOH). Warm ligroine (50 ml.) containing 5.0 g. 2,5-diphenylpyrrole stirred (N atmospheric) 3 hrs. under reflux with 1.0 g. K, the mixture refluxed 30 min. with ClCO2Me, the mixture cooled slightly, stirred with 5 ml. AcOH to remove excess K, the mixture poured into 300 ml. 2:1 H2O-C6H6, and the dried (MgSO4) organic layer evaporated in vacuo yielded 67%

I (R1 = R2 = Ph), m. 100° (ligroine and sublimed at 90-5°/0.04 mm.), λ 292, 224, 202 mμ (ε 17,200, 13,500, 30,500, MeOH). Equimolar amts. of I and III heated (oil bath) in a stream of N 3 hrs. at 160-70° with absorption of C2H2 in aqueous Cu2Cl2NH4OH and the black oily residue distilled at 0.1 mm. gave IV as listed. The filtered and washed C2Cu2 decomposed with 10% HCl and saturated with H2S gave Cu2s corresponding to the evolved C2H2 [R1, R2, number, m.p. (solvent), % yield IV, λ in mμ (ε), τ (number of groups), and % yield C2H2 given]: Me, Me, V, 94° (CCl4), 51, 265 (5990), 6.15 (1), 6.35 (2), 7.57 (2), 30.3; Me, H, VI, 64° (CCl4), 31, 260 (6700), 2.45 (1), 6.06 (3), 6.27 (6), 7.45 (3), 19.0; H, H, VII, 67° (CCl4), 43.5, 251 (9700), 3.10 (2), 6.31 (6), 6.38 (3), 25.0. IV refluxed 2 hrs. in 25 ml. 50% MeOH containing 2.0 g. NaOH, the filtered solns. acidified with concentrated HCl, the precipitated acids air-dried, and esterified at 20° with excess ethereal CH2N2 and diazoethane gave the corresponding pyrrole-3,4-carboxylates (VIII). V(2 g.)yielded 65% VIII (R1 = R2 = Me, R = H), m. 260-5° (decomposition) (50% MeOH), λ 270, 207 mμ (ε 7370, 9950) [R = Et, m. 94-7°, λ 266, 212 mμ (ε 8030, 9450); R = Me, m. 118-19°]. VI (1.3 g.) yielded 81% VIII (R1 = Me, R2 = R = H), m. 230-4° (decomposition), λ 261, 242, 208 mμ (ε 6730, 5300, 9820, MeOH) [R = Et, m. 121°, λ 260, 212 mμ (ε 7240, 9450); R = Me, m. 159°]. VII (2.1 g.) yielded 80% VIII (R = R1 = R2 = H), m. 151-2°, λ 253, 206 mμ (ε 7550, 10350); di-Me ester m. 241-2° Attempted reaction of I(R1 = R2 = Ph) with III resulted in recovery of starting materials. Similar attempted use of maleic anhydride, dimethyl fumarate, Ph2C2, and (NC)2C:C(CN)2 as dienophiles was unsuccessful.

IT 94905-31-4P, Pyrrole-1-carboxylic acid, 2,5-diphenyl-, methyl ester
RL: PREP (Preparation)
(preparation of)

RN 94905-31-4 CAPLUS

CN 1H-Pyrrole-1-carboxylic acid, 2,5-diphenyl-, methyl ester (9CI) (CA INDEX NAME)